STIC Search Report
Biotech-Chem Library

STIC Database Tracking Number: 206718

TO: Rei-Tsang Shiao
Location: REM-5A10/5C18
Art Unit: 1626
Tuesday, November 21, 2006
Case Serial Number: 10/749806

From: Les Henderson
Location: Biotech-Chem Library
REM-1B61
Phone: (571)272-2538

leslie.henderson@uspto.gov

Search Notes

Results can also be viewed via SCORE. http://es/ScoreAccessWeb/

STIC
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STIC SEARCH RESULTS FEEDBACK FORM

Biotech-Chem Library

Questions about the scope or the results of the search? Contact ***the searcher or contact***:

Mary Hale, Information Branch Supervisor
571-272-2507 Remsen 1 A51

Voluntary Results Feedback Form

- *I am an examiner in Workgroup:* ☐ *Example: 1610*
- *Relevant prior art **found**, search results used as follows:*
  - ☐ 102 rejection
  - ☐ 103 rejection
  - ☐ Cited as being of interest.
  - ☐ Helped examiner better understand the invention.
  - ☐ Helped examiner better understand the state of the art in their technology.

  Types of relevant prior art found:
  - ☐ Foreign Patent(s)
  - ☐ Non-Patent Literature
    (journal articles, conference proceedings, new product announcements etc.)
- *Relevant prior art **not found:***
  - ☐ Results verified the lack of relevant prior art (helped determine patentability).
  - ☐ Results were not useful in determining patentability or understanding the invention.

Comments:

Drop off or send completed forms to STIC/Biotech-Chem Library Remsen Bldg.

sira
Search and Information Resources Administration

11-259

FOR OFFICIAL USE ONLY 206718 ACCESS DB # ______
PLEASE PRINT CLEARLY

Scientific and Technical Information Center

SEARCH REQUEST FORM

Requester's Full Name: Robert (Reitsong) Shiao Examiner # : 7952 Date: 1/06/06
Art Unit: 1626 Phone Number: 2-0707 Serial Number: 10/749806
Location (Bldg/Room#): REM (Mailbox #): 5A02 / 5C18 Results Format Preferred (circle): PAPER DISK
****

To ensure an efficient and quality search, please attach a copy of the cover sheet, claims, and abstract or fill out the following:

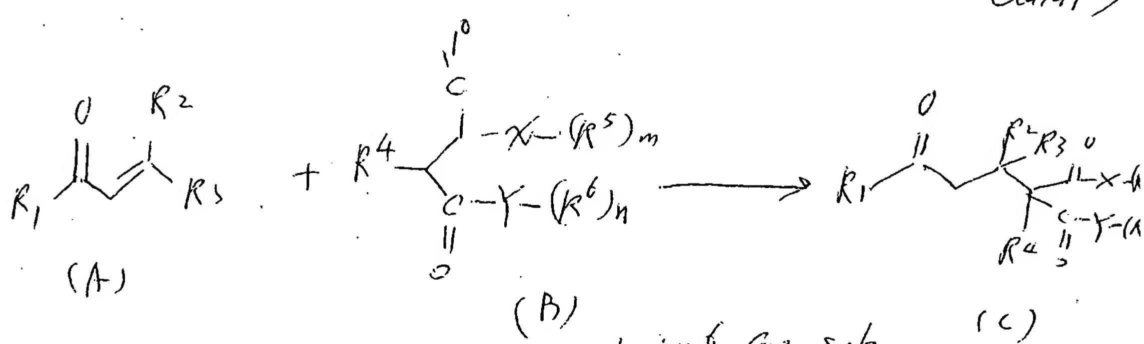
Title of Invention: Process for producing optically active cpd
Inventors (please provide full names): Watanabe et al.

Earliest Priority Date: ______

Search Topic:
Please provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be searched. Include the elected species or structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or utility of the invention. Define any terms that may have a special meaning. Give examples or relevant citations, authors, etc., if known.

For Sequence Searches Only *Please include all pertinent information (parent, child, divisional, or issued patent numbers) along with the appropriate serial number.*

I. Search a process of making cpd (c) by (see claim)



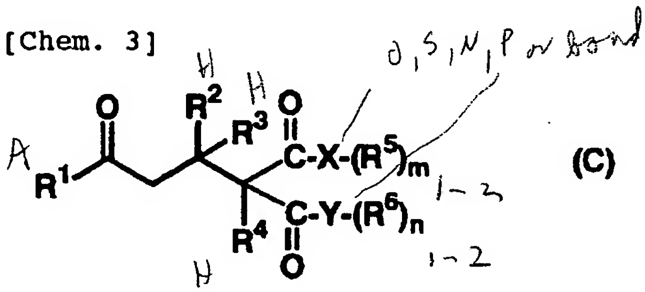
* $R^1 \sim R^6$ are sub.
* X, Y is a bond, O, S, N or P.
* $R_1 \sim R^6$ are sub
* R^1/R^2, R^1/R^3, R^2/R^3 may form a ring

II. Search a process making (R)-3-[bis(ethoxycarbonyl)methyl]cyclopentanone by reacting (see example 8, 9) hexamethylbenzene + 2-cyclopentone → product.

What is claimed is:

1. A process for producing an optically active compound represented by general formula (C)

[Chem. 3]

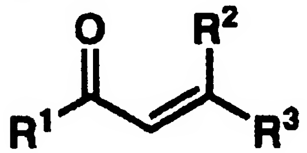


(C)

(in the formula, R^1 denotes an aromatic monocyclic or aromatic polycyclic hydrocarbon group, which may have a substituent, a saturated or unsaturated aliphatic hydrocarbon group or alicyclic hydrocarbon group, which may have a substituent, a heteromonocyclic or heteropolycyclic group, which may have a substituent, or a hydrogen atom, an alkoxy group, or an amino group; R^2 and R^3 independently denote a hydrogen atom, an aromatic monocyclic or aromatic polycyclic hydrocarbon group, which may have a substituent, a saturated or unsaturated aliphatic hydrocarbon group or alicyclic hydrocarbon group, which may have a substituent, or a heteromonocyclic or heteropolycyclic group, which may have a substituent, and R^1 and R^2, R^1 and R^3, or R^2 and R^3 may be bonded to each other to form a ring; may form ring R^4 denotes a hydrogen atom, an aromatic monocyclic or aromatic polycyclic hydrocarbon group, which may have a substituent, a saturated or unsaturated aliphatic hydrocarbon group or alicyclic hydrocarbon group, which may have a substituent, or a heteromonocyclic or heteropolycyclic group, which may have a substituent; R^5 and R^6 independently denote a hydrogen atom, an aromatic monocyclic or aromatic polycyclic hydrocarbon group, which may have a substituent, a saturated or unsaturated aliphatic hydrocarbon group or alicyclic hydrocarbon group, which may have

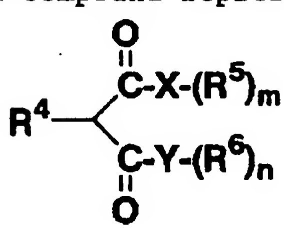
a substituent, or a straight-chain or branched C1 to C20 alkoxy group, and R^4 and R^5, R^4 and R^6, or R^5 and R^6 may be bonded to each other to form a ring; X and Y independently denote a single bond, an oxygen atom, a sulfur atom, a ~~nitrogen atom, or a phosphorus~~ atom; and m and n are independently 1 or 2; when X and/or Y is a single bond, an oxygen atom, or a sulfur atom, m and/or n is 1, and when X and/or Y is a nitrogen atom or a phosphorus atom, m and/or n is 2) by reacting a compound represented by general formula (A)

[Chem. 1]



(A)

(in the formula, R^1, R^2, and R^3 have the same meaning as above) and a compound represented by general formula (B)[Chem. 2]



(B)

(in the formula, R^4, R^5, R^6, X, Y, m, and n have the same meaning as above) with an asymmetric metal complex obtained from an optically active nitrogen-containing compound and a complex of a metal of group VIII of the periodic table.

2. The process for producing an optically active compound according to Claim 1, wherein X and Y of compound (B) according to Claim 1 are both oxygen atoms.

3. The process for producing an optically active compound according to Claim 1, wherein X of compound (B) according to Claim 1 is an oxygen atom and Y is a single bond, or X is a single bond and Y is an oxygen atom.

chromatography (hexane/acetone = 90/10, SiO_2) to give 213 mg (99% yield) of the title compound. The optical purity was measured by HPLC (CHIRALPAK AS manufactured by Daicel Chemical Industries, Ltd., hexane : 2-propanol = 80 : 20, flow rate 1.0 mL/min, detection at 210 nm) and it was found to be 89 %ee.

(Example 8)

Production of (R)-3-[bis(ethoxycarbonyl)methyl] cyclopentanone

Under an atmosphere of argon, 12.6 mg (0.02 mmol, S/C = 50) of Ru[(S,S)-Tsdpen] (hexamethylbenzene), 84 μL (1.0 mmol) of 2-cyclopentenone, 152 μL (1.0 mol) of diethyl malonate, and 1 mL of 2-methyl-2-propanol were placed in a 20 mL Schlenk tube and stirred at 40°C for 24 hours. This solution was purified by flash column chromatography (hexane/acetone = 90/10, SiO_2) to give 233 mg (96% yield) of the title compound. After this was converted into an ethylene ketal derivative by the same procedure as in Example 3, the optical purity was measured by HPLC (CHIRALCEL OD manufactured by Daicel Chemical Industries, Ltd., hexane : 2-propanol = 97 : 3, flow rate 0.5 mL/min, detection at 210 nm) and it was found to be 96 %ee.

(Example 9)

Production of (S)-3-[bis(ethoxycarbonyl)methyl] cyclopentanone

Under an atmosphere of argon, 24.0 mg (0.04 mmol, S/C = 50) of RuH[(R,R)-Tsdpen] (1,3,5-trimethylbenzene), 168 μL (2.0 mmol) of 2-cyclopentenone, 304 μL (2.0 mmol) of diethyl malonate, and 2 mL of acetone were placed in a 20 mL Schlenk tube and stirred at 40°C for 24 hours. This solution was purified by flash column chromatography (hexane/acetone = 90/10, SiO_2) to give 462 mg (95% yield) of the title compound. After this was converted into an ethylene ketal derivative by the same procedure as in Example 3,

the optical purity was measured by HPLC (CHIRALCEL OD manufactured by Daicel Chemical Industries, Ltd., hexane : 2-propanol = 97 : 3, flow rate 0.5 mL/min, detection at 210 nm) and it was found to be 91 %ee.

(Example 10)

Production of 3-[1,1-bis(methoxycarbonyl)ethyl] cyclopentanone

Under an atmosphere of argon, 12.6 mg (0.02 mmol, S/C = 50) of Ru[(S,S)-Tsdpen] (hexamethylbenzene), 84 μL (1.0 mmol) of 2-cyclopentenone, 133 μL (1.0 mmol) of dimethyl methylmalonate, and 1 mL of 2-methyl-2-propanol were placed in a 20 mL Schlenk tube and stirred at 40°C for 24 hours. This solution was purified by flash column chromatography (hexane/acetone = 90/10, SiO_2) to give 54 mg (24% yield) of the title compound. The optical purity was measured by HPLC (CHIRALPAK AS manufactured by Daicel Chemical Industries, Ltd., hexane : 2-propanol = 80 : 20, flow rate 1.5 mL/min, detection at 210 nm) and it was found to be 76 %ee.

(Example 11)

Production of 3-[bis(methoxycarbonyl)methyl]-4, 4-dimethylcyclopentanone

Under an atmosphere of argon, 12.3 mg (0.02 mmol, S/C = 50) of Ru[(S,S)-Tsdpen] (1,2,3,4,5-pentamethylbenzene), 122 μL (1.0 mmol) of 4,4-dimethyl-2-cyclopentenone, 114 μL (1.0 mmol) of dimethyl malonate, and 1 mL of 2-methyl-2-propanol were placed in a 20 mL Schlenk tube and stirred at 40°C for 48 hours. This solution was purified by flash column chromatography (hexane/acetone = 90/10, SiO_2) to give 141 mg (58% yield) of the title compound. After they were converted into an ethylene ketal derivative by the same procedure as in Example 3, the optical purity was measured by HPLC (CHIRALCEL OD manufactured by Daicel Chemical Industries, Ltd.,

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Bib Data Sheet

CONFIRMATION NO. 6518

SERIAL NUMBER	FILING DATE	CLASS	GROUP ART UNIT	ATTORNEY DOCKET NO.
10/749,806	12/31/2003 RULE	558	1626	60542(49811)

APPLICANTS

Masahito Watanabe, Soka-shi, JAPAN;

Kunihiko Murata, Soka-shi, JAPAN;
Takao Ikariya, Tokyo, JAPAN;

** CONTINUING DATA *************************

** FOREIGN APPLICATIONS ********************
JAPAN 2003-9786 01/17/2003
JAPAN 2003-71368 03/17/2003

IF REQUIRED, FOREIGN FILING LICENSE GRANTED
** 03/23/2004

Foreign Priority claimed / 35 USC 119 (a-d) conditions met / Verified and Acknowledged	STATE OR COUNTRY	SHEETS DRAWING	TOTAL CLAIMS	INDEPENDENT CLAIMS
Foreign Priority claimed: ☒ yes ☐ no 35 USC 119 (a-d) conditions met: ☒ yes ☐ no ☐ Met after Allowance Verified and Acknowledged: Examiner's Signature / Initials	JAPAN	0	9	1

ADDRESS
EDWARDS & ANGELL, LLP
P.O. Box 9169
Boston , MA
02209

TITLE
Process for producing optically active compound

FILING FEE RECEIVED	FEES: Authority has been given in Paper No. _________ to charge/credit DEPOSIT ACCOUNT No. _________ for following:	☐ All Fees ☐ 1.16 Fees (Filing) ☐ 1.17 Fees (Processing Ext. of time) ☐ 1.18 Fees (Issue)

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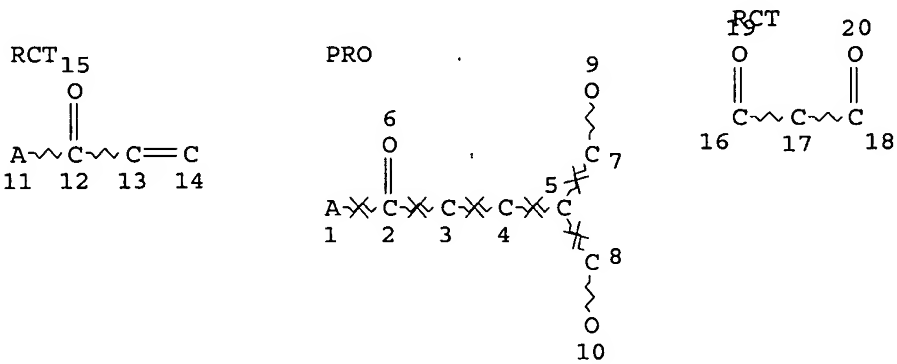


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CONNECT IS E1   RC AT   15
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DEFAULT ECLEVEL IS LIMITED

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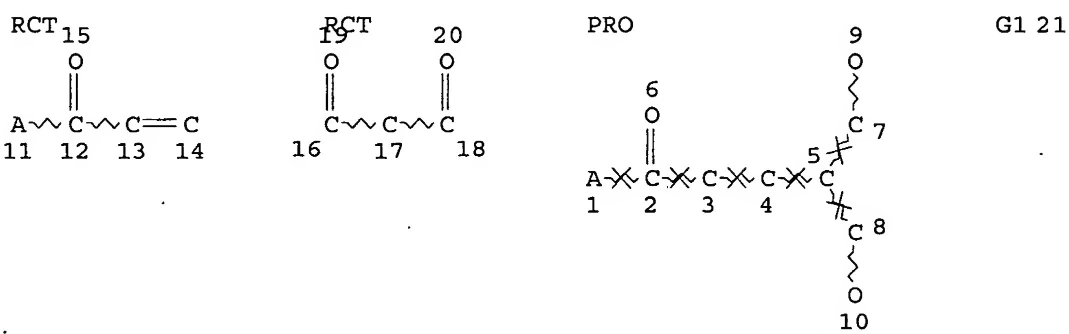


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Pt @30

VAR G1=22/23/24/25/26/27/28/29/30
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11/21/2006


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100.0% DONE      31 VERIFIED      31 HIT RXNS                 7 DO
CS
SEARCH TIME: 00.00.02


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L20 ANSWER 1 OF 7 CASREACT COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 136:37336 CASREACT

TITLE: Tandem anionic Michael addition/radical cyclizations: a new and efficient strategy for the synthesis of functionalized cyclopentanes

AUTHOR(S): Jahn, Ullrich

CORPORATE SOURCE: Institut fur Organische Chemie, TU Braunschweig, Braunschweig, D-38106, Germany

SOURCE: Chemical Communications (Cambridge, United Kingdom) (2001), (17), 1600-1601

CODEN: CHCOFS; ISSN: 1359-7345

PUBLISHER: Royal Society of Chemistry

DOCUMENT TYPE: Journal

LANGUAGE: English

CLASSIFICATION: 24-4 (Alicyclic Compounds)

ABSTRACT:
The combination of anionic Michael addition of lithium ester enolates with radical 5-exo cyclizations through single electron transfer (SET) oxidation gives highly functionalized cyclopentanes.

SUPPL. TERM: electron transfer cyclization Michael addn ester enolate

INDEX TERM: Electron transfer
(preparation of functionalized cyclopentanes via tandem anionic Michael addition/radical cyclization)

INDEX TERM: Cyclization
(radical; preparation of functionalized cyclopentanes via tandem anionic Michael addition/radical cyclization)

INDEX TERM: Addition reaction
Michael reaction
(stereoselective; preparation of functionalized cyclopentanes via tandem anionic Michael addition/radical cyclization)

INDEX TERM: 2564-83-2, TEMPO
ROLE: CAT (Catalyst use); RCT (Reactant); RACT (Reactant or reagent); USES (Uses)
(prepn of functionalized cyclopentanes via tandem anionic Michael addition/radical cyclization)

INDEX TERM: 11077-24-0, Ferrocenium hexafluorophosphate
ROLE: CAT (Catalyst use); RCT (Reactant); RACT (Reactant or reagent); USES (Uses)
(preparation of functionalized cyclopentanes via tandem anionic Michael addition/radical cyclization)

INDEX TERM: 94-41-7 1462-12-0 5292-53-5 377752-09-5 377752-10-8 377752-11-9 377752-12-0 377752-13-1
ROLE: RCT (Reactant); RACT (Reactant or reagent)
(preparation of functionalized cyclopentanes via tandem anionic Michael addition/radical cyclization)

INDEX TERM: 377752-26-6P
ROLE: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of functionalized cyclopentanes via tandem anionic Michael addition/radical cyclization)

INDEX TERM: 377752-14-2P 377752-15-3P 377752-16-4P
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377752-20-0P 377752-21-1P 377752-22-2P
377752-23-3P 377752-24-4P 377752-25-5P
377752-27-7P 377752-28-8P 377752-29-9P
377752-30-2P 377752-31-3P 377752-32-4P
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377752-39-1P 377752-40-4P 377752-41-5P
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377752-48-2P 377752-49-3P 377752-50-6P
377752-51-7P 377752-52-8P 377752-53-9P
377752-54-0P 377752-55-1P 377752-56-2P
377752-57-3P 377752-58-4P 377752-59-5P
377752-60-8P 379738-76-8P 379738-77-9P
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ROLE: SPN (Synthetic preparation); PREP (Preparation)
(preparation of functionalized cyclopentanes via tandem anionic Michael addition/radical cyclization)

REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD.

REFERENCE(S):
(1) Bernardi, A; Gazz Chim Ital 1995, V125, P539 CAPLUS
(2) Boger, D; J Org Chem 1997, V62, P8875 CAPLUS
(3) Cohen, T; Tetrahedron 1993, V49, P7931 CAPLUS
(4) Curran, D; Comprehensive Organic Synthesis 1991, V4, P715
(5) Curran, D; Comprehensive Organic Synthesis 1991, V4, P779
(6) Curran, D; Stereochemistry of Radical Reactions 1996
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(10) Heathcock, C; Modern Synthetic Methods 1992, V6, P1 CAPLUS

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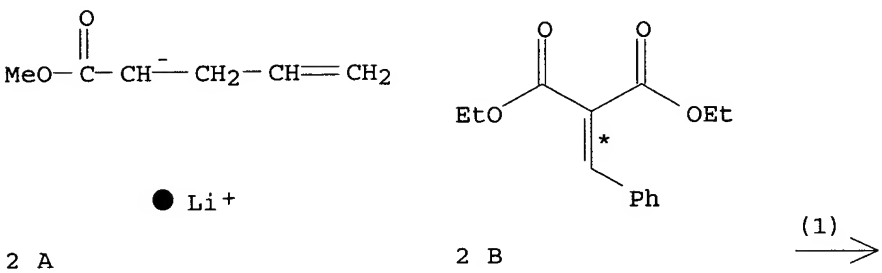
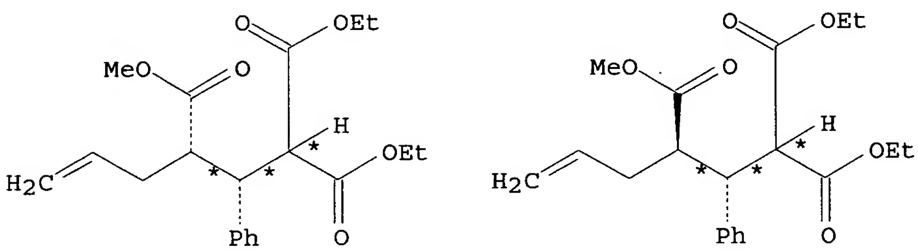
(15) Oare, D; Top Stereochem 1989, V19, P227 CAPLUS
(16) Sibi, M; J Am Chem Soc 1999, V121, P7517 CAPLUS

RX(1) OF 17 2 A + 2 B ===> C + D



2 A

2 B



C
YIELD 96%(87)

D
YIELD 96%(13)

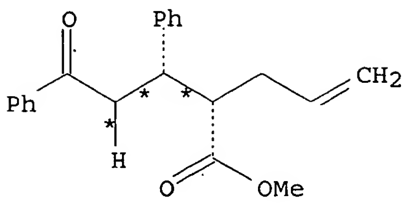
RX(1) RCT A 377752-09-5, B 5292-53-5

STAGE(1)
RGT E 680-31-9 HMPT
SOL 109-99-9 THF

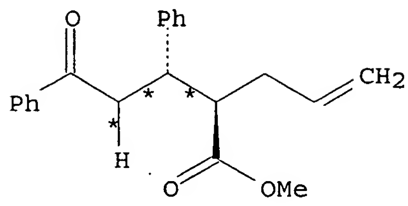
STAGE(2)
RGT F 7732-18-5 Water

PRO C 377752-14-2, D 377752-15-3
NTE stereoselective

RX(2) OF 17 2 A + 2 B ===> D + C



I
YIELD 84%(88)



J
YIELD 84%(12)

RX(3) RCT A 377752-09-5, H 94-41-7

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SOL 109-99-9 THF

STAGE(2)
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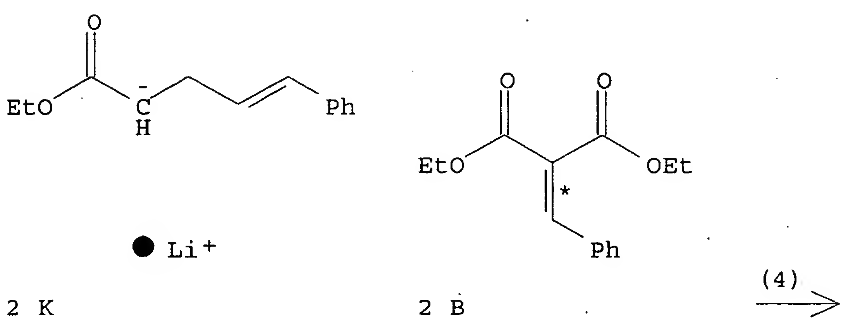
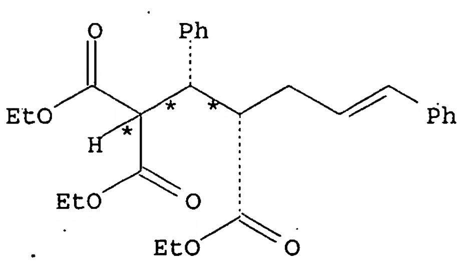
PRO I 377752-16-4, J 377752-17-5
NTE stereoselective

RX(4) OF 17 2 K + 2 B ===> L + M

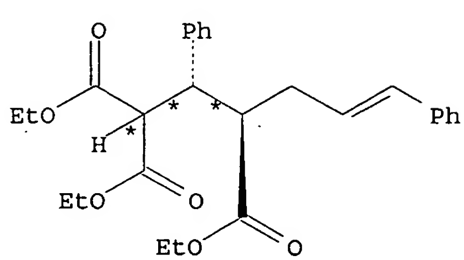


2 K

2 B

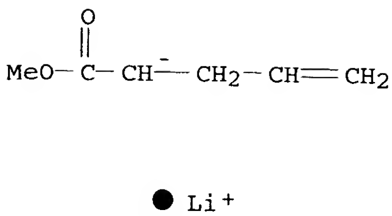


L
YIELD 95%(90)

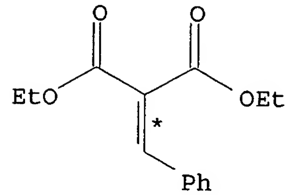


M
YIELD 95%(10)

RX(4) RCT K 377752-10-8, B 5292-53-5

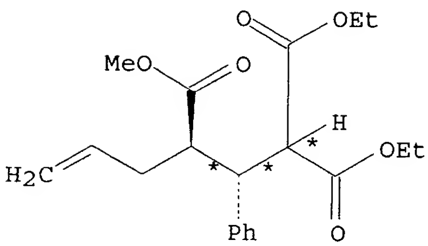


2 A

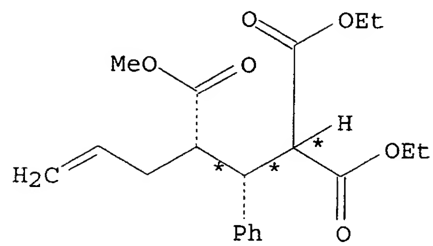


2 B

(2) →



D
YIELD 58%(65)



C
YIELD 58%(35)

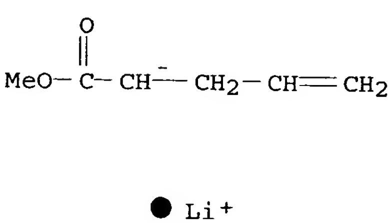
RX(2) RCT A 377752-09-5, B 5292-53-5

STAGE(1)
SOL 109-99-9 THF

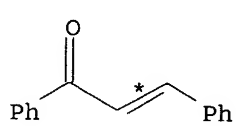
STAGE(2)
RGT F 7732-18-5 Water

PRO D 377752-15-3, C 377752-14-2
NTE stereoselective

RX(3) OF 17 2 A + 2 H ===> I + J



2 A



2 H

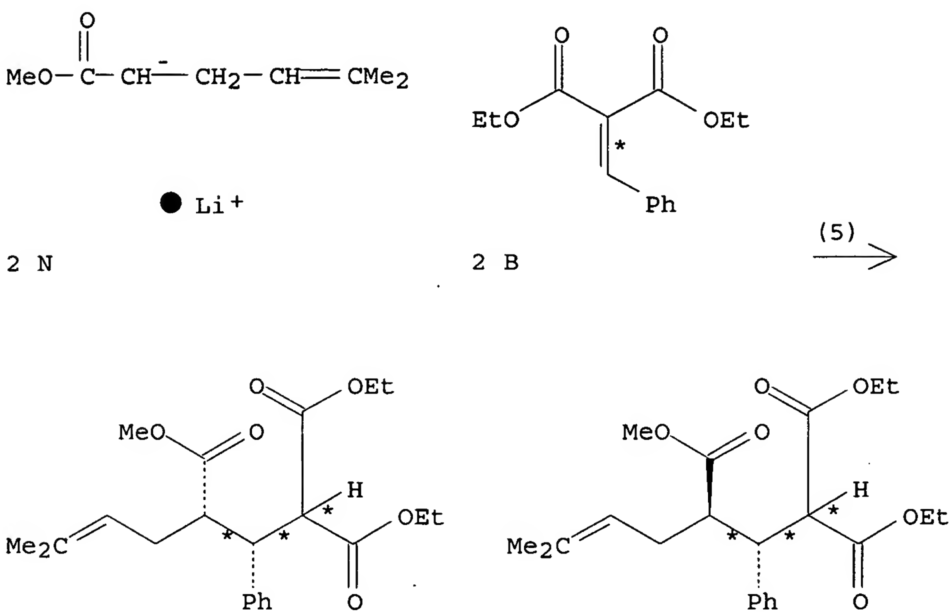
(3) →

STAGE(1)
RGT E 680-31-9 HMPT
SOL 109-99-9 THF

STAGE(2)
RGT F 7732-18-5 Water

PRO L 377752-18-6, M 377752-19-7
NTE stereoselective

RX(5) OF 17 2 N + 2 B ===> O + P



2 N 2 B

O
YIELD 77%(92)

P
YIELD 77%(8)

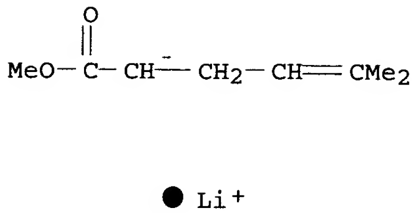
RX(5) RCT N 377752-12-0, B 5292-53-5

STAGE(1)
RGT E 680-31-9 HMPT
SOL 109-99-9 THF

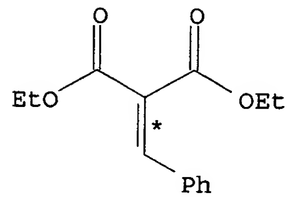
STAGE(2)
RGT F 7732-18-5 Water

PRO O 377752-20-0, P 377752-21-1
NTE stereoselective

RX(6) OF 17 2 N + 2 B ===> P + O

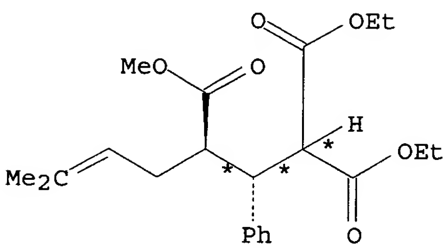


2 N

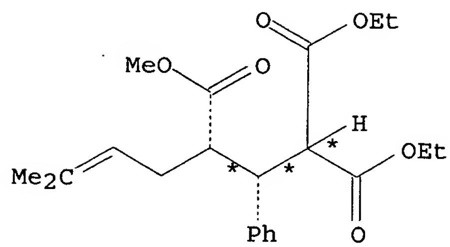


2 B

(6) →



P
YIELD 90%(69)



O
YIELD 69%(31)

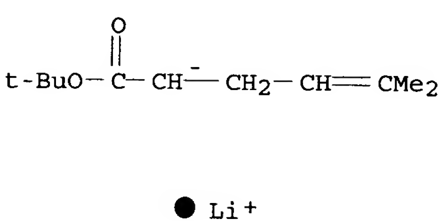
RX(6) RCT N 377752-12-0, B 5292-53-5

STAGE(1)
SOL 109-99-9 THF

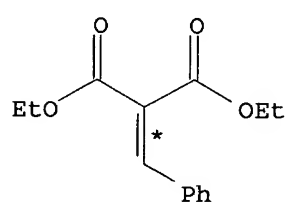
STAGE(2)
RGT F 7732-18-5 Water

PRO P 377752-21-1, O 377752-20-0
NTE stereoselective

RX(7) OF 17 2 Q + 2 B ===> R + S

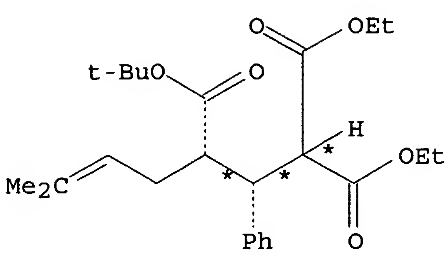


2 Q

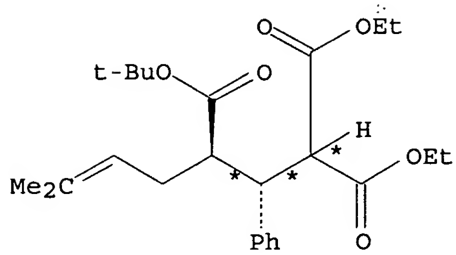


2 B

(7) →



R
YIELD 93%(92)



S
YIELD 93%(8)

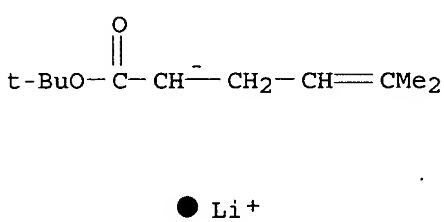
RX(7) RCT Q 377752-13-1, B 5292-53-5

STAGE(1)
RGT E 680-31-9 HMPT
SOL 109-99-9 THF

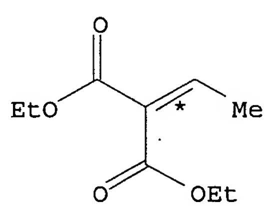
STAGE(2)
RGT F 7732-18-5 Water

PRO R 377752-22-2, S 377752-23-3
NTE stereoselective

RX(8) OF 17 2 Q + 2 T ===> U + V

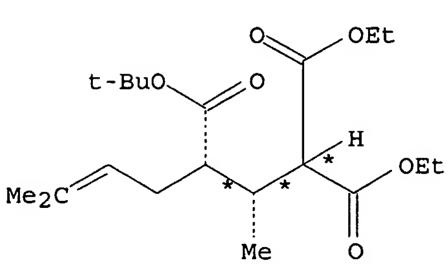


2 Q

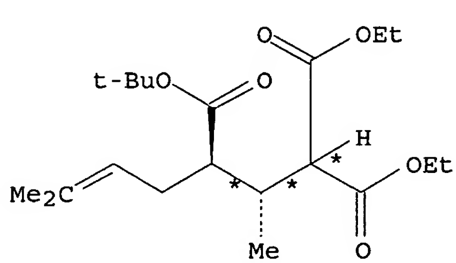


2 T

(8) ⟶



U
YIELD 92%(82)



V
YIELD 92%(18)

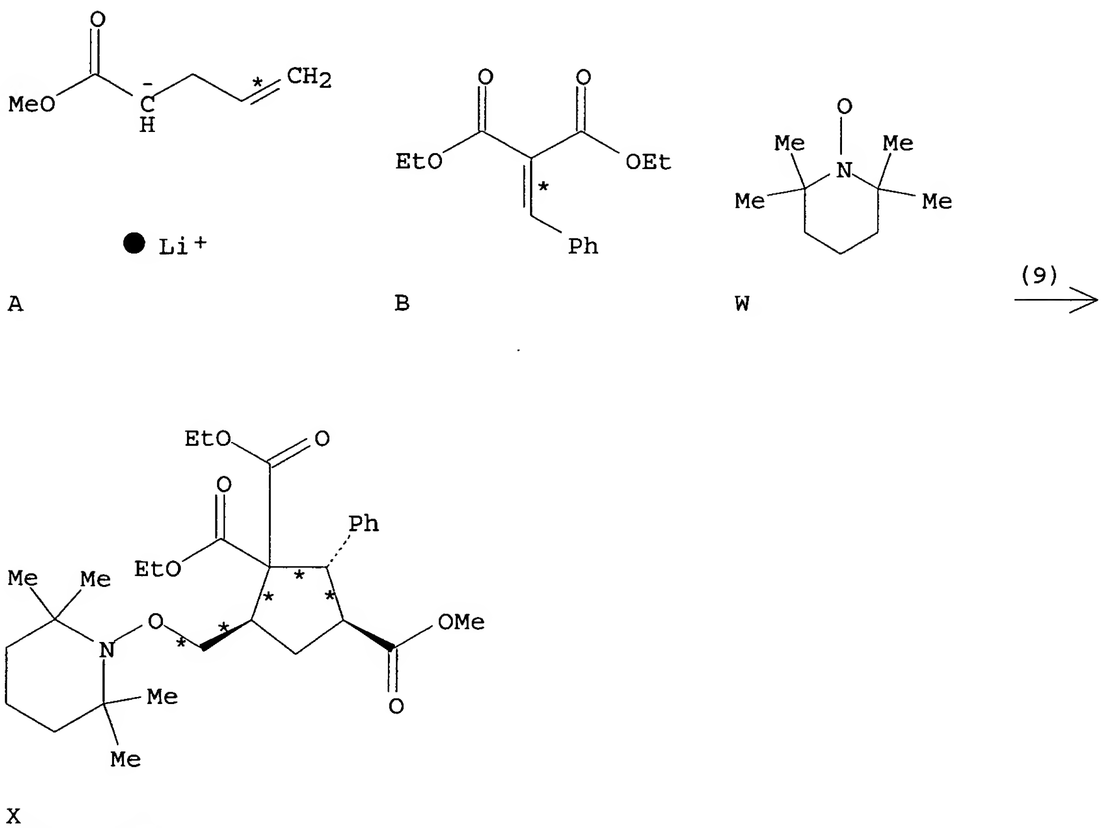
RX(8) RCT Q 377752-13-1, T 1462-12-0

STAGE(1)
RGT E 680-31-9 HMPT
SOL 109-99-9 THF

STAGE(2)
RGT F 7732-18-5 Water

PRO U 377752-24-4, V 377752-25-5
NTE stereoselective

RX(9) OF 17 A + B + W ===> X



YIELD 71%

RX(9) RCT A 377752-09-5

STAGE(1)
RGT Y 75-31-0 i-PrNH2, Z 109-72-8 BuLi, E 680-31-9 HMPT
SOL 109-99-9 THF, 110-54-3 Hexane

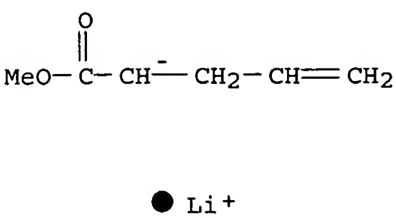
STAGE(2)
RCT B 5292-53-5

STAGE(3)
RCT W 2564-83-2
RGT AA 11077-24-0 Ferrocenium PF6

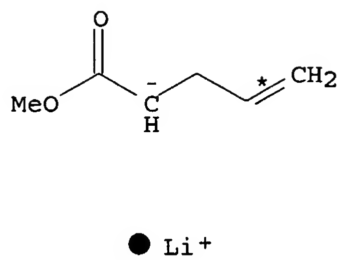
STAGE(4)
RGT F 7732-18-5 Water

PRO X 377752-26-6

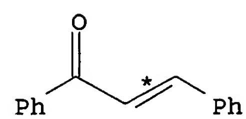
RX(10) OF 17 5 A + 5 H + 5 W ===> AC + AD + AE + AF + AG



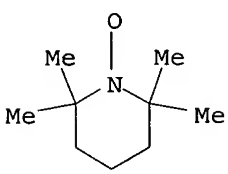
4 A



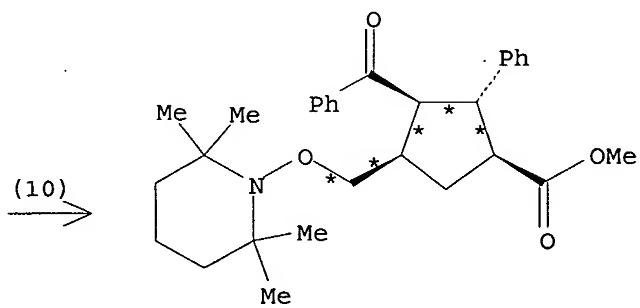
A



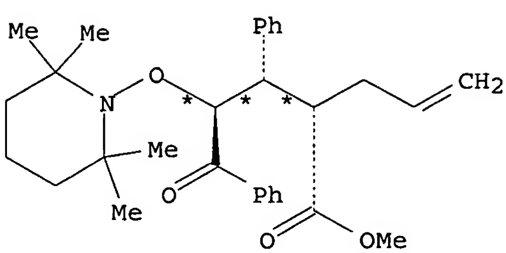
5 H



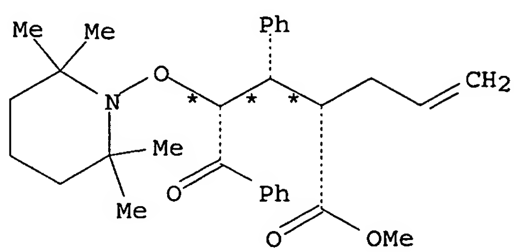
5 W



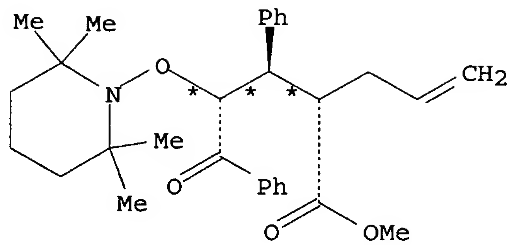
AC
YIELD 53%(88)



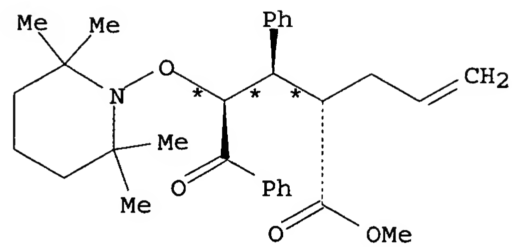
AD



AE



AF



AG

RX(10) RCT A 377752-09-5

STAGE(1)
RGT Y 75-31-0 i-PrNH2, Z 109-72-8 BuLi, E 680-31-9 HMPT
SOL 109-99-9 THF, 110-54-3 Hexane

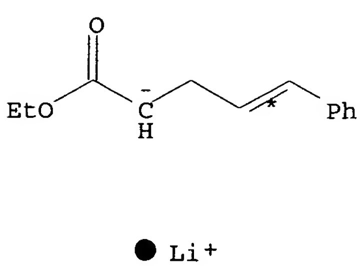
STAGE(2)
RGT H 94-41-7

STAGE(3)
RCT W 2564-83-2
RGT AA 11077-24-0 Ferrocenium PF6

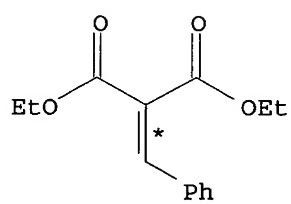
STAGE(4)
RGT F 7732-18-5 Water

PRO AC 377752-31-3, AD 377752-27-7, AE 377752-28-8, AF 377752-29-9, AG 377752-30-2
NTE isomeric methyl 2-allyl-5-oxo-3,5-diphenyl-4-(2,2,6,6-tetramethylpiperidin-1-yloxy)pentanoates 25% overall yield

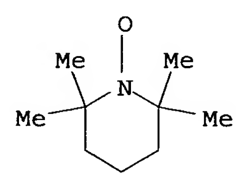
RX(11) OF 17 2 K + 2 B + 2 W ===> **AH** +
AI



2 K

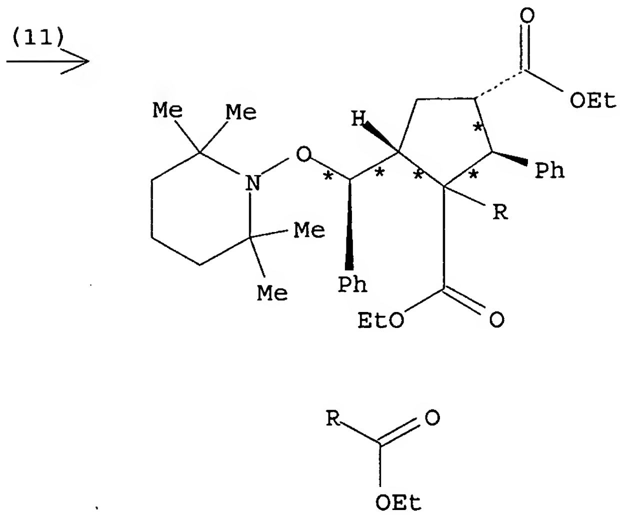


2 B

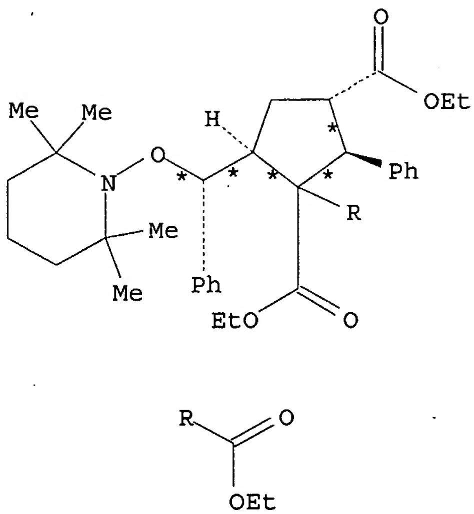


2 W

(11)



AH
YIELD 87%(53)



AI
YIELD 87%(37)

RX(11)   RCT K 377752-10-8

    STAGE(1)
        RGT Y 75-31-0 i-PrNH2, Z 109-72-8 BuLi, E 680-31-9 HMPT
        SOL 109-99-9 THF, 110-54-3 Hexane

    STAGE(2)
        RCT B **5292-53-5**

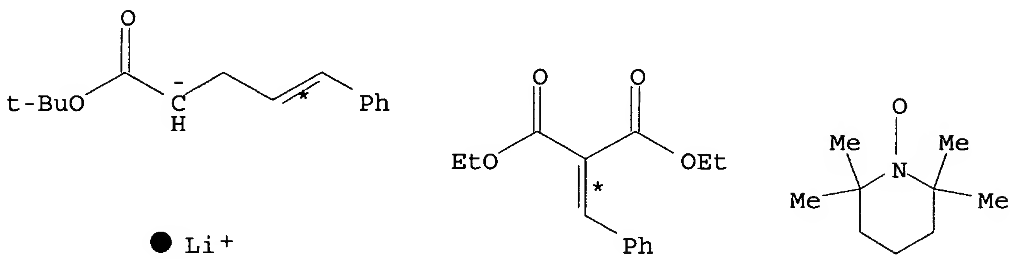
    STAGE(3)

RCT W 2564-83-2
RGT AA **11077-24-0** Ferrocenium PF6

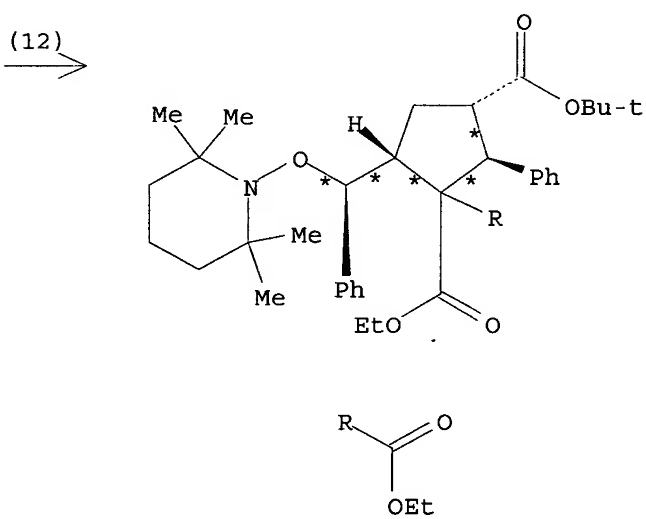
STAGE(4)
RGT F 7732-18-5 Water

PRO AH **377752-32-4**, AI 377752-33-5
NTE other products also detected

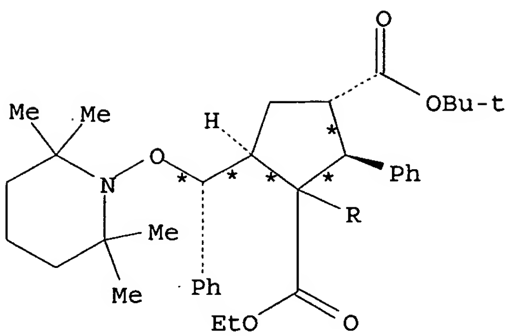
RX(12) OF 17 2 AJ + 2 **B** + 2 W ===> **AK** +
AL

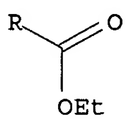


2 AJ 2 B 2 W



AK
YIELD 86%(67)





AL
YIELD 29%

RX(12) RCT AJ 377752-11-9

STAGE(1)
RGT Y 75-31-0 i-PrNH2, Z 109-72-8 BuLi, E 680-31-9 HMPT
SOL 109-99-9 THF, 110-54-3 Hexane

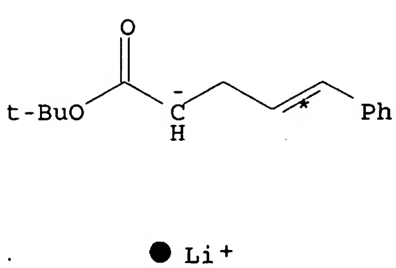
STAGE(2)
RCT B **5292-53-5**

STAGE(3)
RCT W 2564-83-2
RGT AA **11077-24-0** Ferrocenium PF6

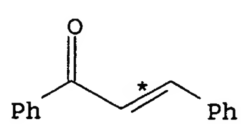
STAGE(4)
RGT F 7732-18-5 Water

PRO AK **377752-34-6**, AL 377752-35-7
NTE other products also detected

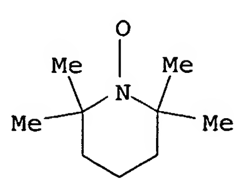
RX(13) OF 17 5 AJ + 5 H + 5 W ===> AM + AN + AO + AP +
AQ



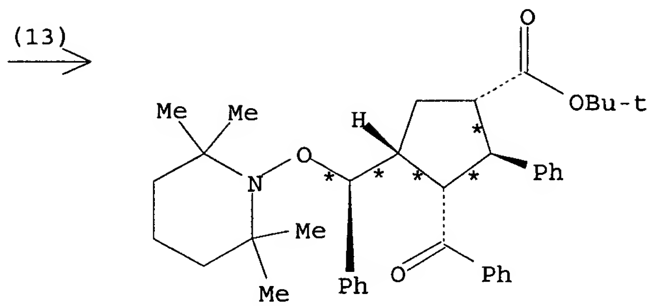
5 AJ



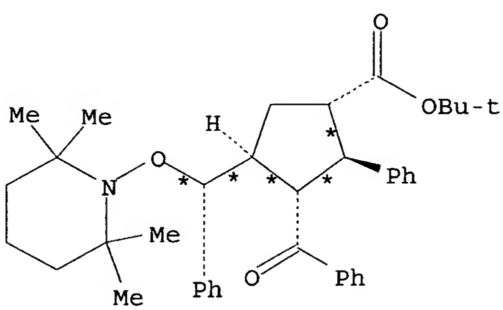
5 H



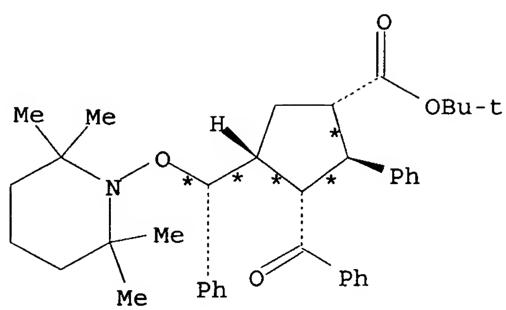
5 W



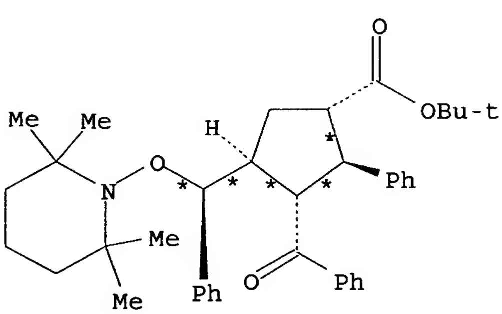
AM
YIELD 61%(68)



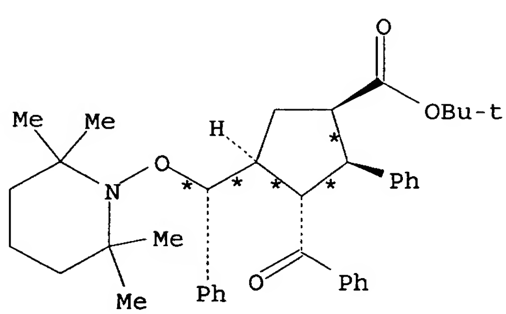
AN
YIELD 67%(13)



AO
YIELD 61%(13)



AP
YIELD 67%(6)



AQ
YIELD 1%

RX(13) RCT AJ 377752-11-9

STAGE(1)
RGT Y 75-31-0 i-PrNH2, Z 109-72-8 BuLi, E 680-31-9 HMPT

SOL 109-99-9 THF, 110-54-3 Hexane

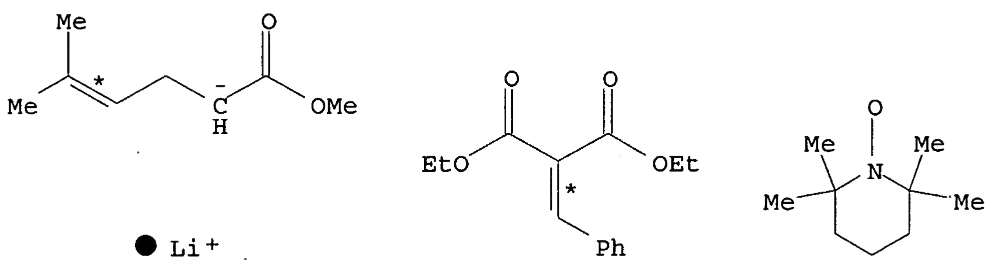
STAGE(2)
RCT H 94-41-7

STAGE(3)
RCT W 2564-83-2
RGT AA 11077-24-0 Ferrocenium PF6

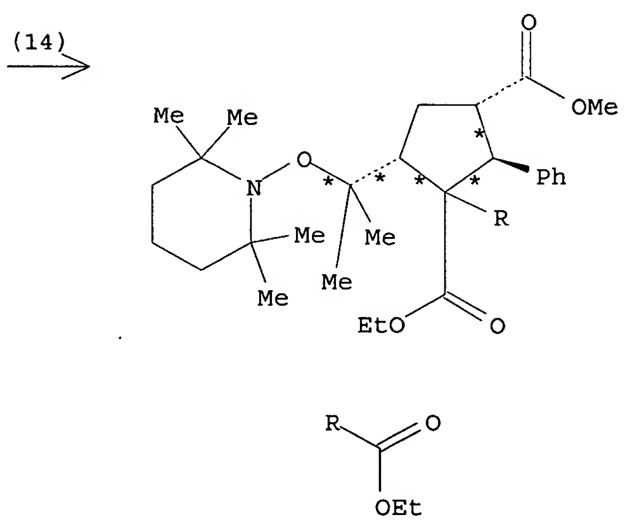
STAGE(4)
RGT F 7732-18-5 Water

PRO AM 377752-36-8, AN 377752-38-0, AO 377752-37-9, AP 377752-39-1, AQ 377752-40-4

RX(14) OF 17 N + B + W ===> AR



N B W



AR
YIELD 82%(64)

RX(14) RCT N 377752-12-0

STAGE(1)

RGT Y 75-31-0 i-PrNH2, Z 109-72-8 BuLi, E 680-31-9 HMPT
SOL 109-99-9 THF, 110-54-3 Hexane

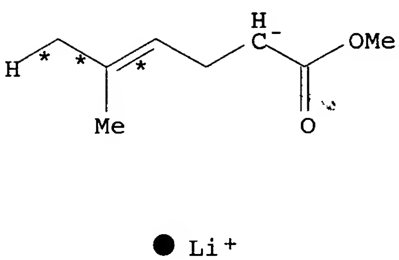
STAGE(2)
RCT B 5292-53-5

STAGE(3)
RCT W 2564-83-2
RGT AA 11077-24-0 Ferrocenium PF6

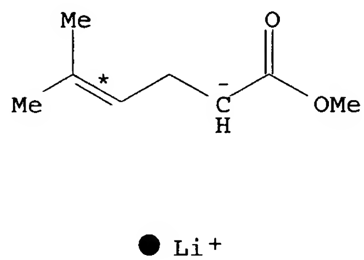
STAGE(4)
RGT F 7732-18-5 Water

PRO AR 377752-41-5
NTE other product also detected

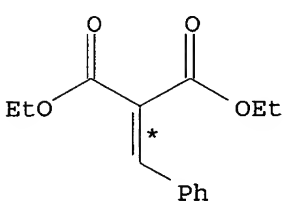
RX(15) OF 17 6 N + 6 **B** + **AA** ===>
AS + AT + AU + AV + AW + AX



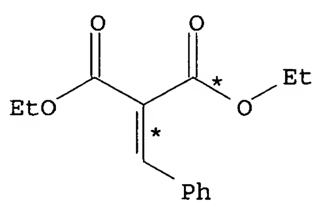
2 N



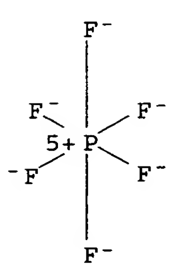
4 N



5 B



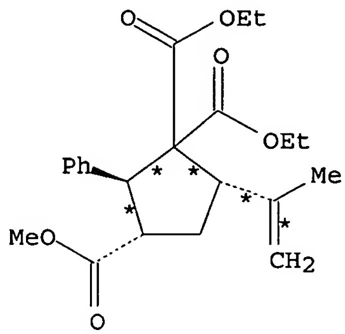
B



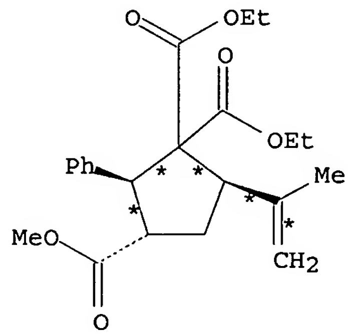
AA: CM 1

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT
*

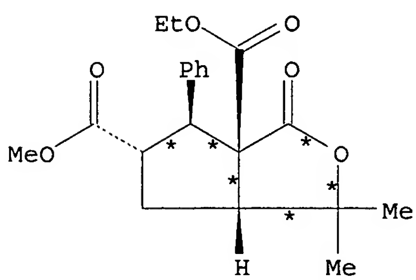
(15) →



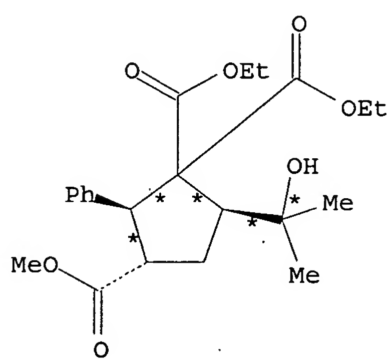
AS
YIELD 51%(75)



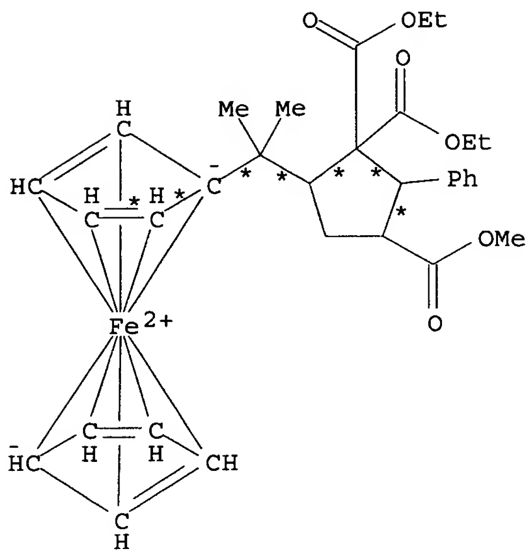
AT
YIELD 51%(25)



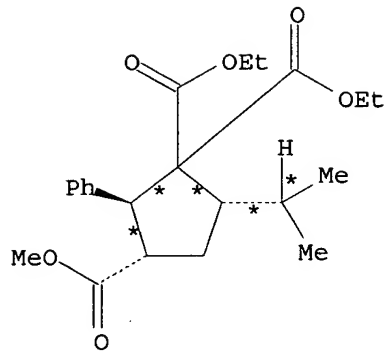
AU
YIELD 9%



AV
YIELD 5%



AW
YIELD 10%(67)



AX
YIELD 2%

RX(15) RCT N 377752-12-0

STAGE(1)
RGT Y 75-31-0 i-PrNH2, Z 109-72-8 BuLi, E 680-31-9 HMPT
SOL 109-99-9 THF, 110-54-3 Hexane

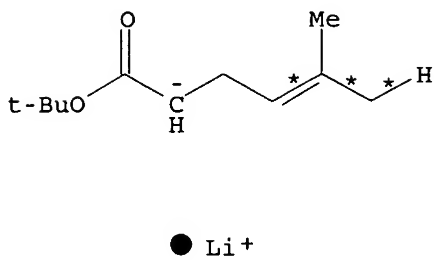
STAGE(2)
RCT B **5292-53-5**

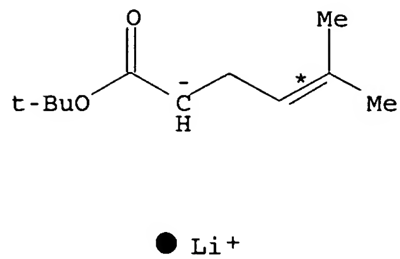
STAGE(3)
RCT AA **11077-24-0**

STAGE(4)
RGT F 7732-18-5 Water

PRO AS **377752-43-7**, AT 377752-44-8, AU 377752-47-1, AV 377752-46-0, AW 379738-76-8, AX 377752-45-9
NTE other product also detected

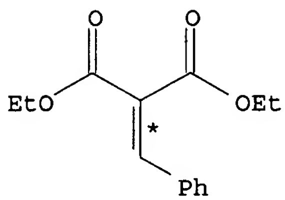
RX(16) OF 17 6 Q + 6 **B** + 2 **AA** ===>
AY + AZ + BA + BB + BC + BD

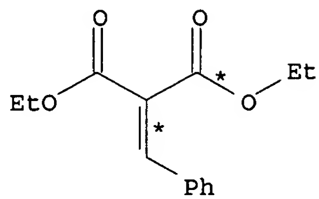




Q

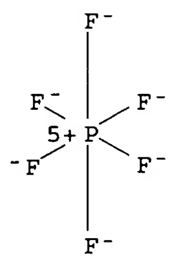
5 Q





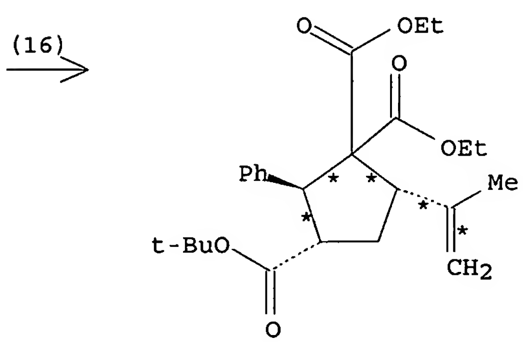
4 B

2 B

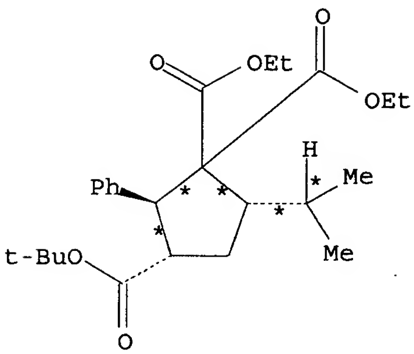


2 AA: CM 1

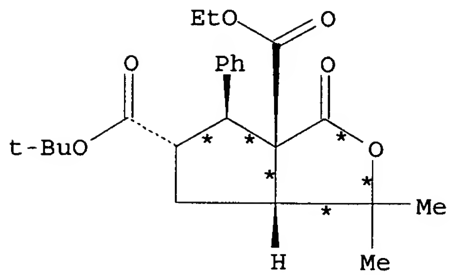
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT
*



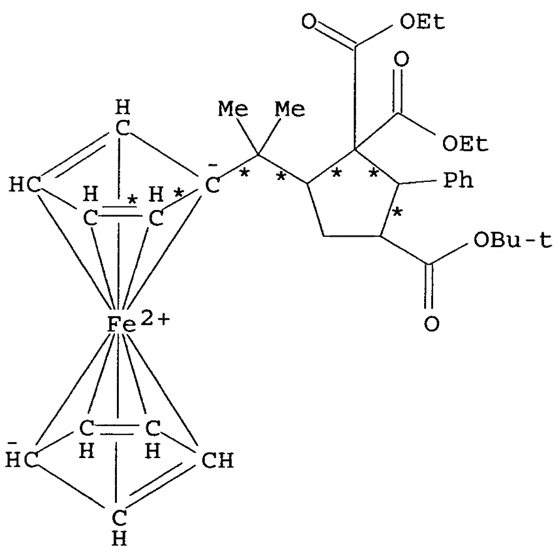
AY
YIELD 54%(94)



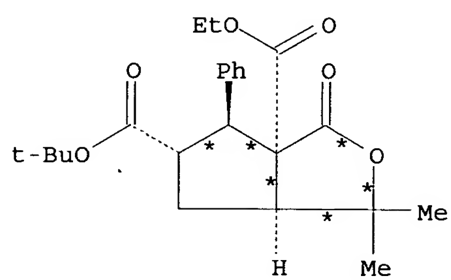
AZ
YIELD 12%



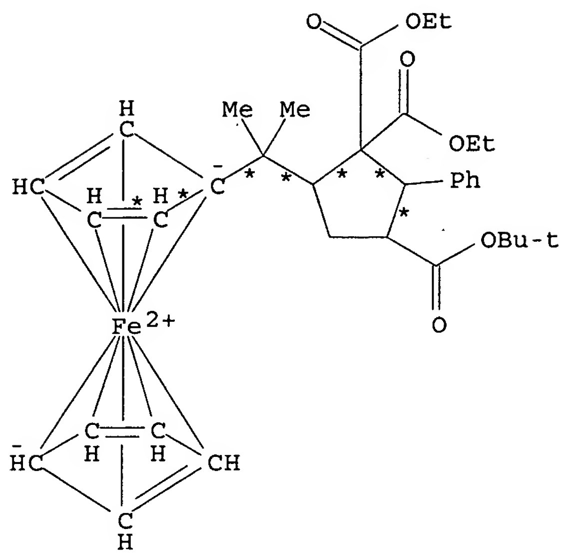
BA
YIELD 11%(75)



BB
YIELD 8%(74)



BC
YIELD 11%(25)



BD
YIELD 8%(26)

RX(16) RCT Q 377752-13-1

STAGE(1)
RGT Y 75-31-0 i-PrNH2, Z 109-72-8 BuLi, E 680-31-9 HMPT
SOL 109-99-9 THF, 110-54-3 Hexane

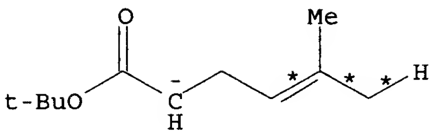
STAGE(2)
RCT B **5292-53-5**

STAGE(3)
RCT AA **11077-24-0**
RGT BE 865-47-4 t-BuOK
SOL 109-99-9 THF

STAGE(4)
RGT F 7732-18-5 Water

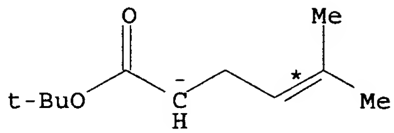
PRO AY **377752-48-2**, AZ 377752-49-3, BA 377752-50-6, BB 379738-77-9, BC 377752-51-7, BD 380153-16-2
NTE other product also detected

RX(17) OF 17 11 Q + 11 **T** + 2 **AA** ===>
BF + BG + BH + BI + BJ + BK + BL + BM + BN + BO + BP



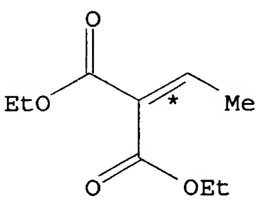
● Li+

4 Q

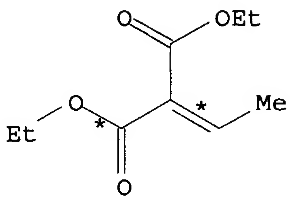


● Li+

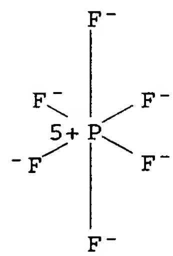
7 Q



7 T



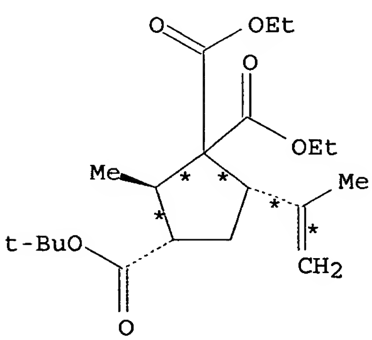
4 T



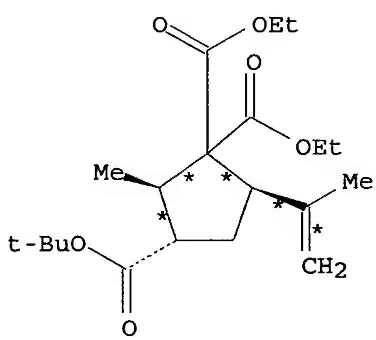
2 AA: CM 1

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT
*

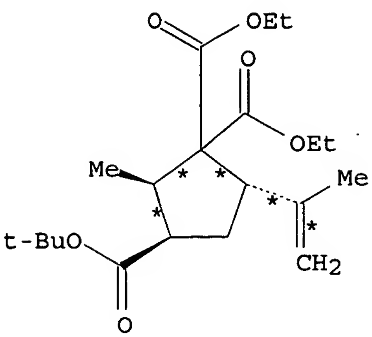
(17) →



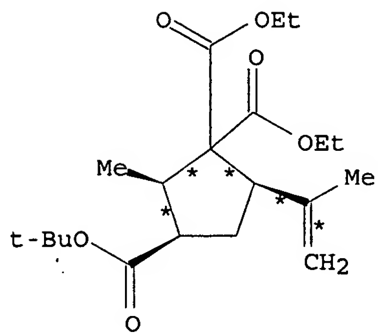
BF
YIELD 54%(71)



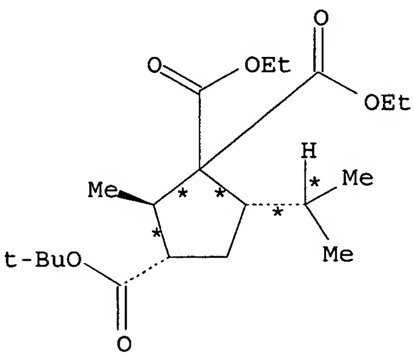
BG
YIELD 54%(18)



BH
YIELD 54%(8)



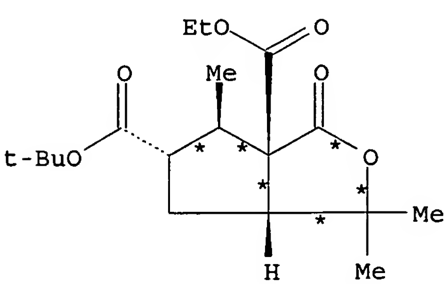
BI
YIELD 54%(3)



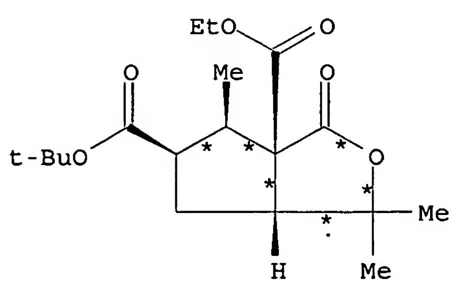
BJ
YIELD 3%

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT
*

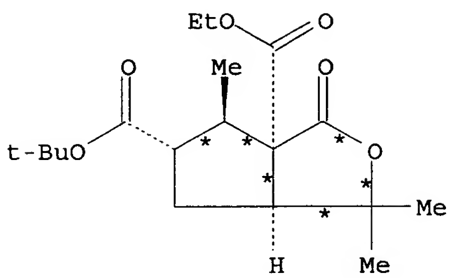
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT
*



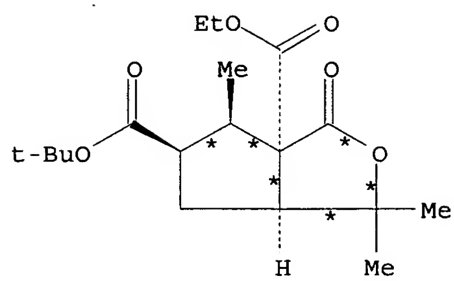
BM



BN



BO



BP

RX(17) RCT Q 377752-13-1

STAGE(1)
RGT Y 75-31-0 i-PrNH2, Z 109-72-8 BuLi, E 680-31-9 HMPT
SOL 109-99-9 THF, 110-54-3 Hexane

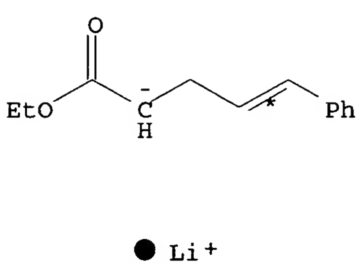
STAGE(2)
RCT T **1462-12-0**

STAGE(3)
RCT AA **11077-24-0**
RGT BE 865-47-4 t-BuOK
SOL 109-99-9 THF

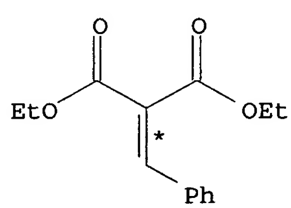
STAGE(4)
RGT F 7732-18-5 Water

PRO BF **377752-52-8**, BG 377752-53-9, BH 377752-54-0, BI 377752-55-1, BJ 377752-56-2, BK 380153-18-4, BL 379738-78-0, BM 377752-57-3, BN 377752-58-4, BO 377752-59-5, BP 377752-60-8
NTE other product also detected

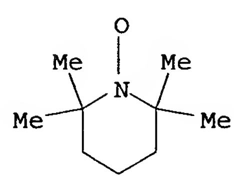
RX(11) OF 17 2 K + 2 **B** + 2 W ===> **AH** + AI



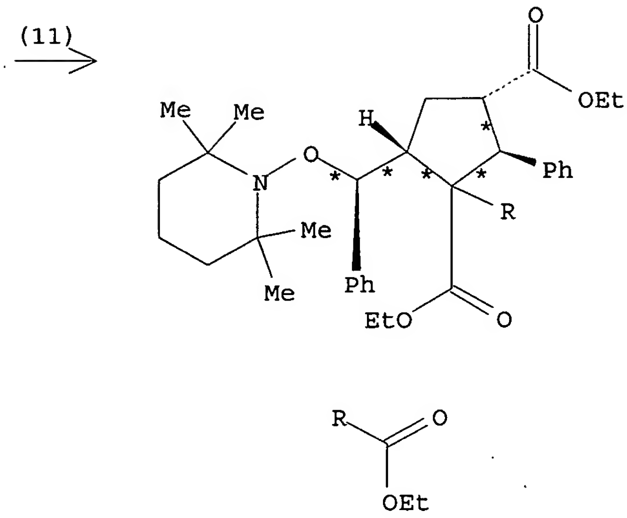
2 K



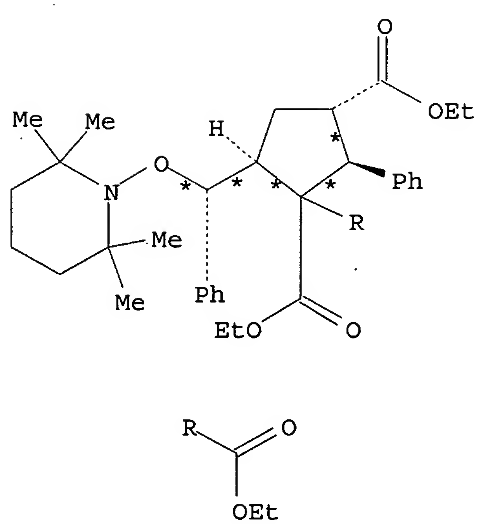
2 B



2 W



AH
YIELD 87%(53)



AI
YIELD 87%(37)

RX(11) RCT K 377752-10-8

STAGE(1)
RGT Y 75-31-0 i-PrNH2, Z 109-72-8 BuLi, E 680-31-9 HMPT
SOL 109-99-9 THF, 110-54-3 Hexane

STAGE(2)
RCT B **5292-53-5**

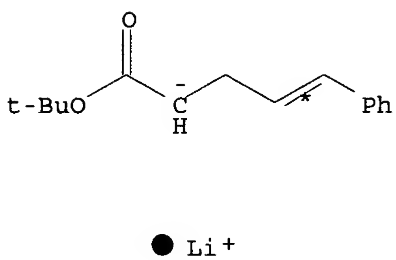
STAGE(3)

RCT W 2564-83-2
RGT AA **11077-24-0** Ferrocenium PF6

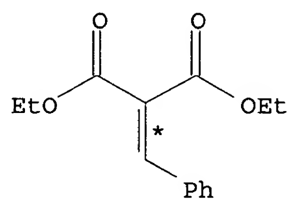
STAGE(4)
RGT F 7732-18-5 Water

PRO AH **377752-32-4**, AI 377752-33-5
NTE other products also detected

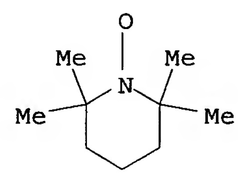
RX(12) OF 17 2 AJ + 2 **B** + 2 W ===> **AK** +
AL



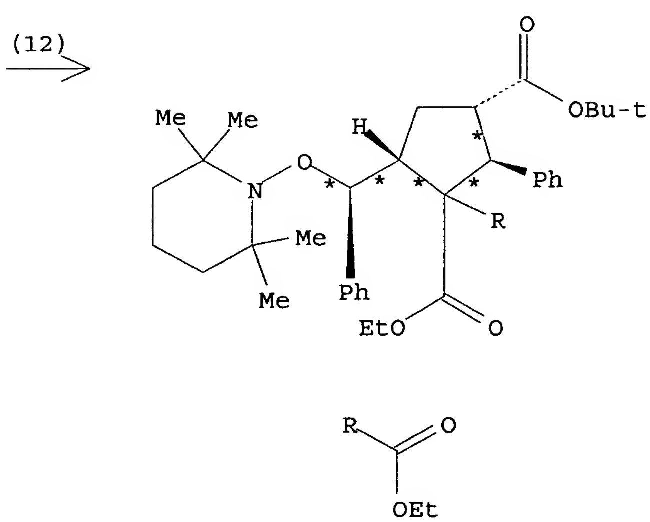
2 AJ



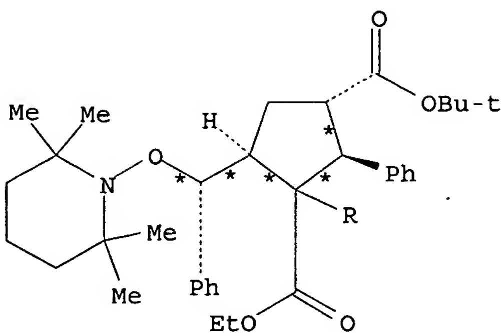
2 B

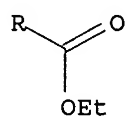


2 W



AK
YIELD 86%(67)





AL
YIELD 29%

RX(12) RCT AJ 377752-11-9

STAGE(1)
RGT Y 75-31-0 i-PrNH2, Z 109-72-8 BuLi, E 680-31-9 HMPT
SOL 109-99-9 THF, 110-54-3 Hexane

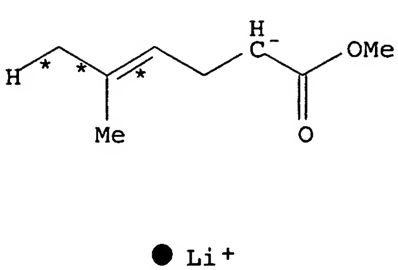
STAGE(2)
RCT B **5292-53-5**

STAGE(3)
RCT W 2564-83-2
RGT AA **11077-24-0** Ferrocenium PF6

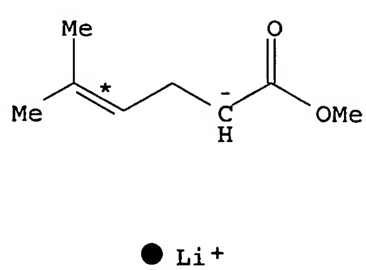
STAGE(4)
RGT F 7732-18-5 Water

PRO AK **377752-34-6**, AL 377752-35-7
NTE other products also detected

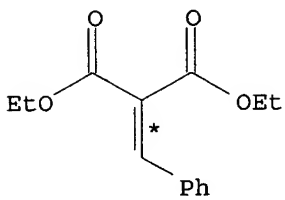
RX(15) OF 17 6 N + 6 **B** + **AA** ===>
AS + AT + AU + AV + AW + AX



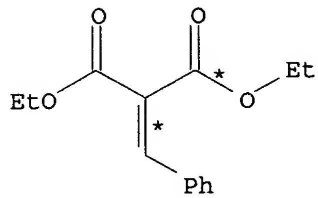
2 N



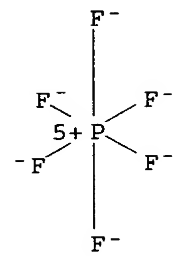
4 N



5 B



B



AA: CM 1

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT
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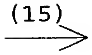
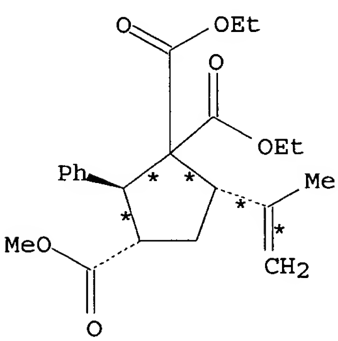
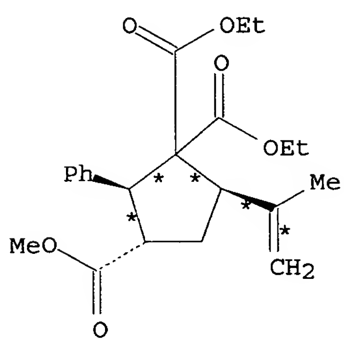
(15)

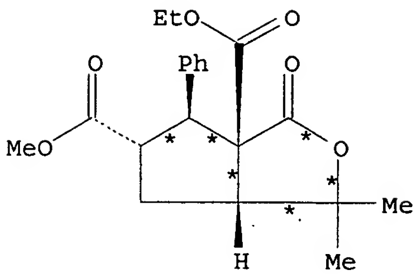




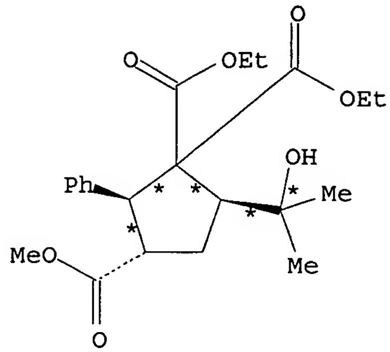
AS
YIELD 51%(75)



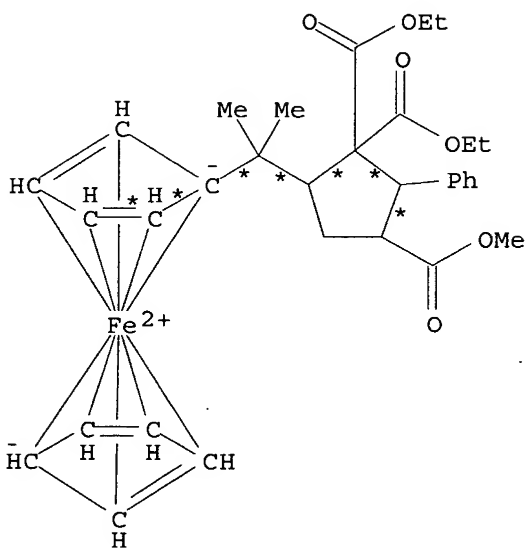
AT
YIELD 51%(25)



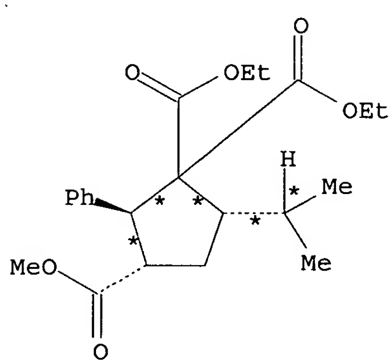
AU
YIELD 9%



AV
YIELD 5%



AW
YIELD 10%(67)



AX
YIELD 2%

RX(15) RCT N 377752-12-0

STAGE(1)
RGT Y 75-31-0 i-PrNH2, Z 109-72-8 BuLi, E 680-31-9 HMPT
SOL 109-99-9 THF, 110-54-3 Hexane

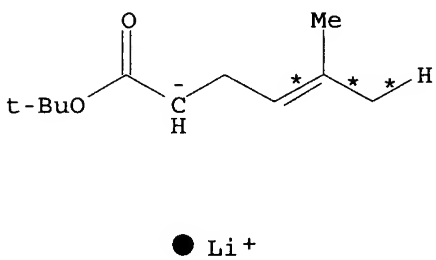
STAGE(2)
RCT B **5292-53-5**

STAGE(3)
RCT AA **11077-24-0**

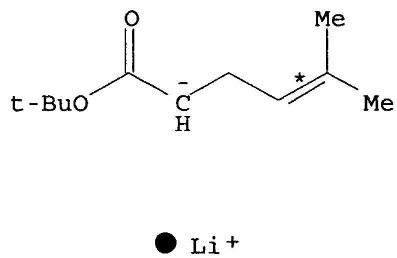
STAGE(4)
RGT F 7732-18-5 Water

PRO AS **377752-43-7**, AT 377752-44-8, AU
377752-47-1, AV 377752-46-0, AW 379738-76-8, AX
377752-45-9
NTE other product also detected

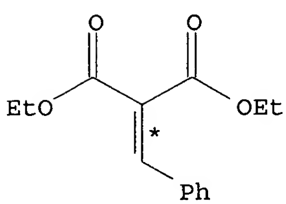
RX(16) OF 17 6 Q + 6 **B** + 2 **AA** ===>
AY + AZ + BA + BB + BC + BD



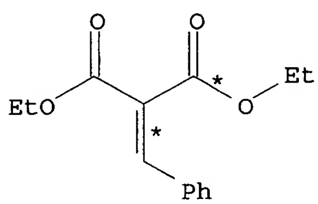
Q



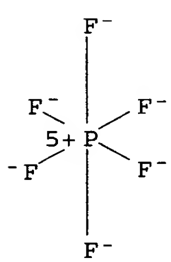
5 Q



4 B



2 B



2 AA: CM 1

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT
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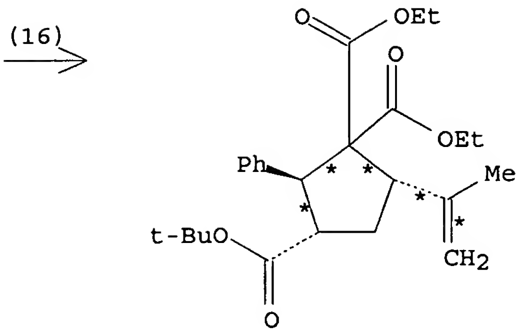
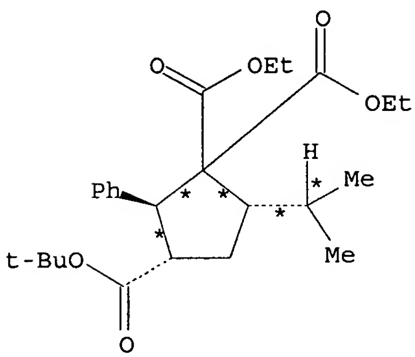
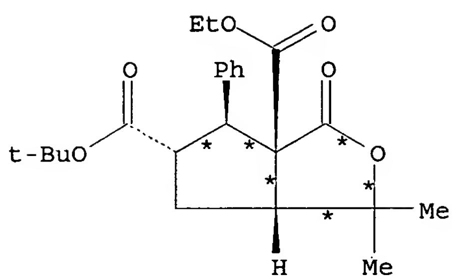


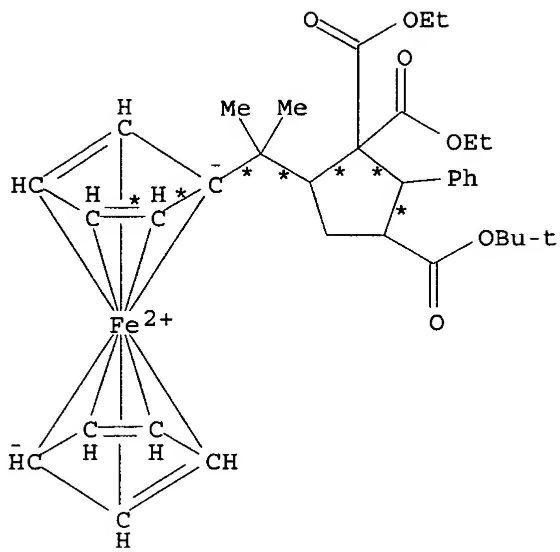
AY
YIELD 54%(94)



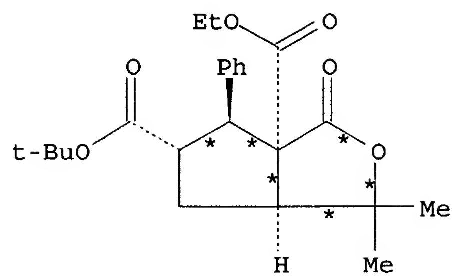
AZ
YIELD 12%



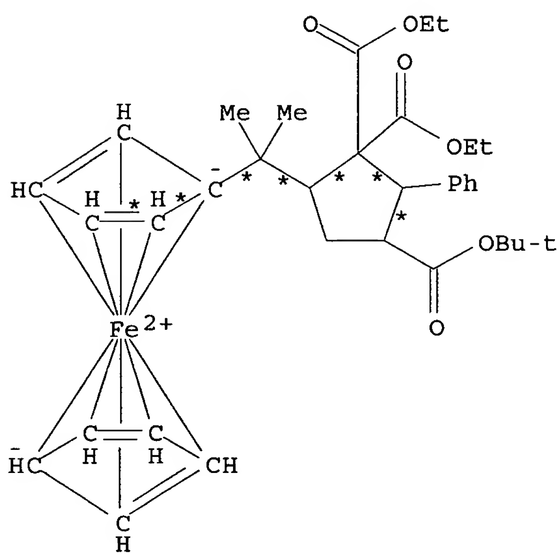
BA
YIELD 11%(75)



BB
YIELD 8%(74)



BC
YIELD 11%(25)



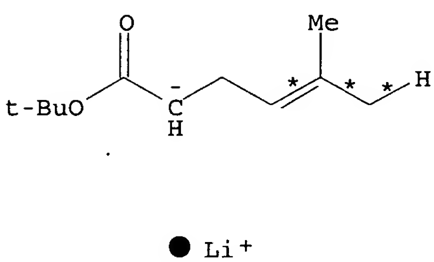
BD
YIELD 8%(26)

RX(16) RCT Q 377752-13-1

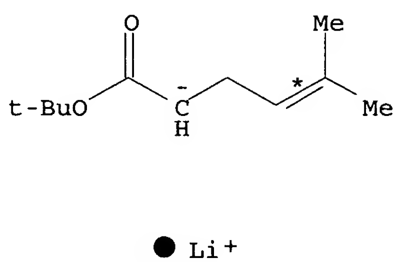
STAGE(1)
RGT Y 75-31-0 i-PrNH2, Z 109-72-8 BuLi, E 680-31-9 HMPT
SOL 109-99-9 THF, 110-54-3 Hexane

STAGE(2)
RCT B **5292-53-5**

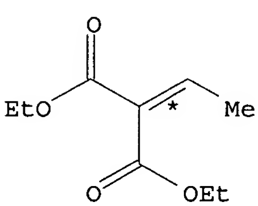
```
    STAGE(3)
       RCT  AA 11077-24-0
       RGT  BE 865-47-4 t-BuOK
       SOL  109-99-9 THF

    STAGE(4)
       RGT  F 7732-18-5 Water

  PRO  AY 377752-48-2, AZ 377752-49-3, BA
       377752-50-6, BB 379738-77-9, BC 377752-51-7, BD
       380153-16-2
  NTE  other product also detected

RX(17) OF 17    11 Q  +  11 T  +  2 AA  ===>
       BF  +  BG  +  BH  +  BI  +  BJ  +  BK  +  BL  +  BM
       +  BN  +  BO  +  BP
```



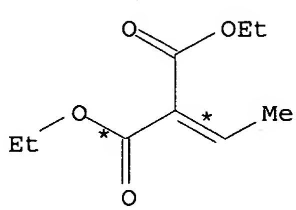
4 Q



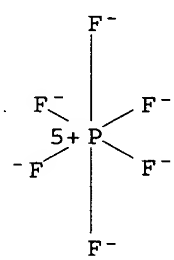
7 Q



7 T



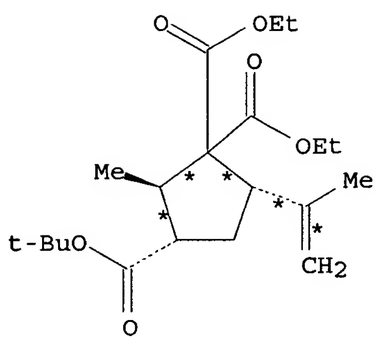
4 T



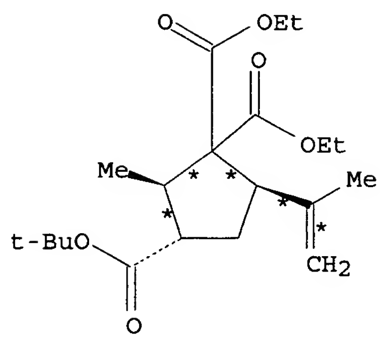
2 AA: CM 1

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

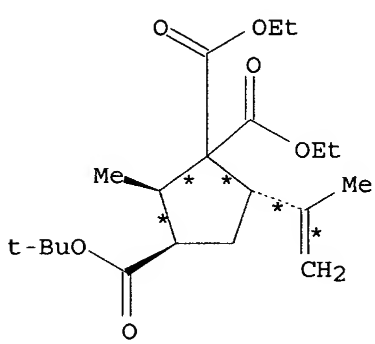
$\xrightarrow{(17)}$



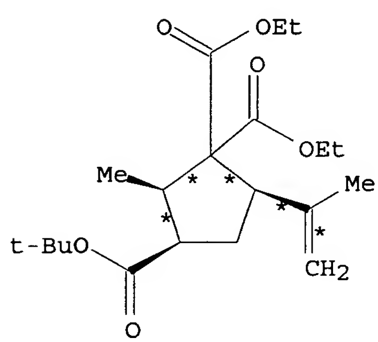
BF
YIELD 54%(71)



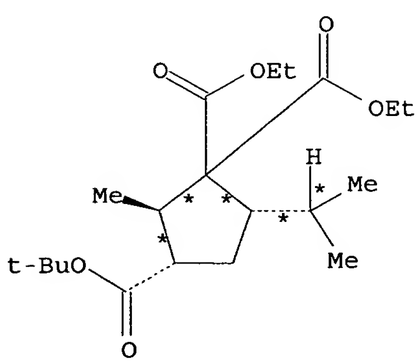
BG
YIELD 54%(18)



BH
YIELD 54%(8)



BI
YIELD 54%(3)



BJ
YIELD 3%

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT
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* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT
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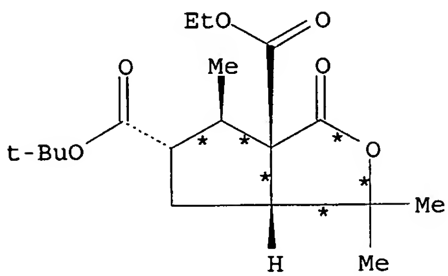

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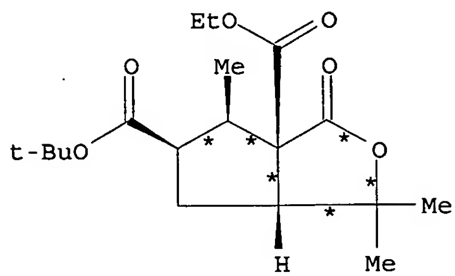

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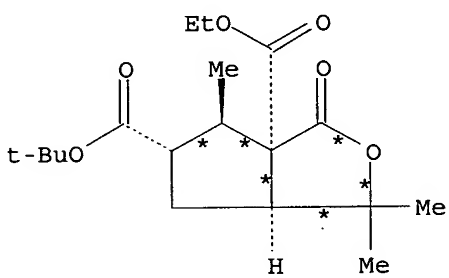

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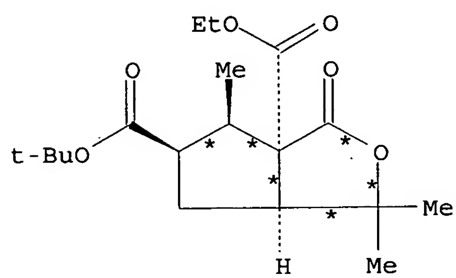

BP

RX(17) RCT Q 377752-13-1

STAGE(1)
RGT Y 75-31-0 i-PrNH2, Z 109-72-8 BuLi, E 680-31-9 HMPT
SOL 109-99-9 THF, 110-54-3 Hexane

STAGE(2)
RCT T **1462-12-0**

STAGE(3)
RCT AA **11077-24-0**
RGT BE 865-47-4 t-BuOK
SOL 109-99-9 THF

STAGE(4)
RGT F 7732-18-5 Water

PRO BF **377752-52-8**, BG 377752-53-9, BH 377752-54-0, BI 377752-55-1, BJ 377752-56-2, BK 380153-18-4, BL 379738-78-0, BM 377752-57-3, BN 377752-58-4, BO 377752-59-5, BP 377752-60-8
NTE other product also detected

L20 ANSWER 2 OF 7 CASREACT COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 134:237626 CASREACT
TITLE: Carbon-carbon bond forming reactions of N-bound transition metal α-cyanocarbanions: a mechanistic probe for catalytic Michael reactions of nitriles
AUTHOR(S): Naota, Takeshi; Tannna, Akio; Murahashi, Shun-Ichi
CORPORATE SOURCE: Department of Chemistry, Graduate School of Engineering Science, Osaka University, Machikaneyama, Toyondaka, Osaka, 560-8531, Japan
SOURCE: Chemical Communications (Cambridge) (2001), (1), 63-64
CODEN: CHCOFS; ISSN: 1359-7345
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
CLASSIFICATION: 29-13 (Organometallic and Organometalloidal Compounds)
Section cross-reference(s): 22

ABSTRACT:
N-Bound α-cyanocarbanion complexes Ru+Cp(NCCH-R1)(PPh3)2 1 react with electron deficient olefins to afford the conjugate adduct Ru+Cp(NCC-R1CHR2CR3R4)(PPh3)2 2, kinetic studies of which revealed that complex 1-catalyzed Michael reactions of nitriles proceed via transformation of 1 to 2 and subsequent ligand exchange with nitriles.

SUPPL. TERM: ruthenium catalyst Michael reaction nitrile alkene; carbon carbon bond formation ruthenium cyanocarbanion catalyst

INDEX TERM: Addition reaction kinetics
(Michael reaction kinetics; of ruthenium cyanocarbanion catalyzed Michael reaction of alkenes with nitriles)

INDEX TERM: Michael reaction
(kinetics; of ruthenium cyanocarbanion catalyzed Michael reaction of alkenes with nitriles)

INDEX TERM: Reaction mechanism
(of ruthenium cyanocarbanion catalyzed Michael reaction of alkenes with nitriles)

INDEX TERM: Alkenes, reactions
Nitriles, reactions
ROLE: RCT (Reactant); RACT (Reactant or reagent)
(ruthenium cyanocarbanion catalyzed Michael reaction of alkenes with nitriles)

INDEX TERM: Michael reaction catalysts
(ruthenium cyanocarbanion; for Michael addition of nitriles with olefins)

INDEX TERM: Carbanions
ROLE: CAT (Catalyst use); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(ruthenium cyanocarbanions; conjugate addition reaction with electron deficient olefins)

INDEX TERM: 6626-84-2
ROLE: RCT (Reactant); RACT (Reactant or reagent)
(Michael reaction with ruthenium carbanions)

INDEX TERM: 7605-28-9
ROLE: RCT (Reactant); RACT (Reactant or reagent)
(conjugate addition of ruthenium carbanions)

INDEX TERM: 17041-60-0, Dimethyl ethylidenemalonate
293767-54-1 330598-53-3
ROLE: RCT (Reactant); RACT (Reactant or reagent)
(conjugate addition to olefins)

INDEX TERM: 264130-83-8
ROLE: CAT (Catalyst use); RCT (Reactant); RACT (Reactant or reagent); USES (Uses)
(conjugate addition to olefins, and catalyst for Michael reactions of nitriles)

INDEX TERM: 330598-57-7P
ROLE: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(preparation and catalyst for Michael reactions of nitriles)

INDEX TERM: 623-43-8
(preparation of)

INDEX TERM: 107-13-1, Acrylonitrile, reactions 625-33-2, Pent-3-en-2-one 2700-22-3, Benzylidenemalononitrile
ROLE: RCT (Reactant); RACT (Reactant or reagent)
(preparation of)

INDEX TERM: 330598-54-4P 330598-55-5P 330598-56-6P
330598-58-8P 330598-59-9P 330598-60-2P
330598-61-3P
ROLE: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD.

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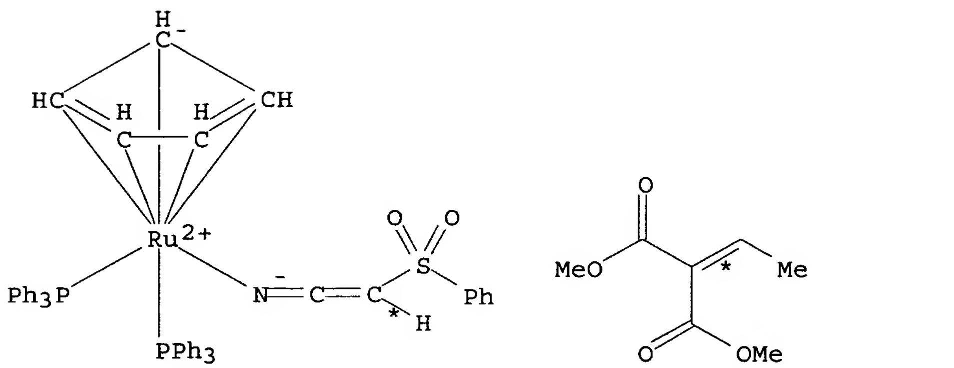
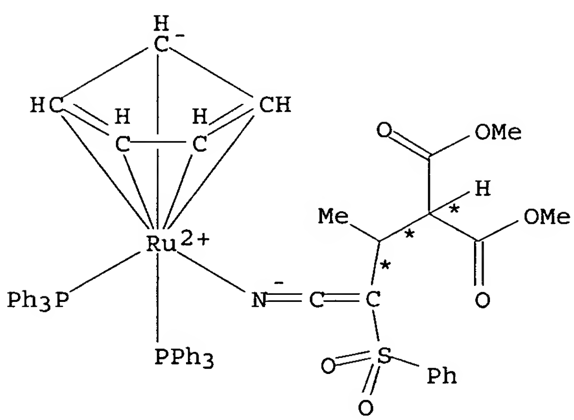
RX(1) OF 8 A + B ===> C



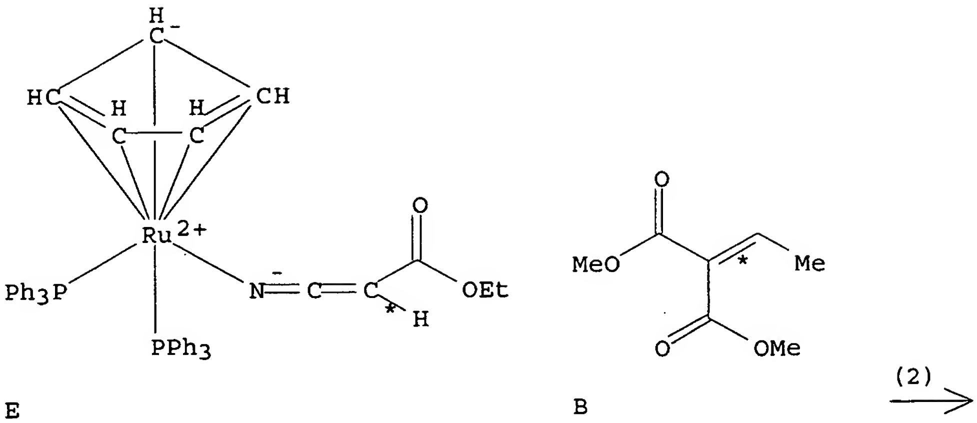
A B



C
YIELD 99%

RX(1) RCT A 264130-83-8, B 17041-60-0
PRO C 330598-54-4
SOL 71-43-2 Benzene

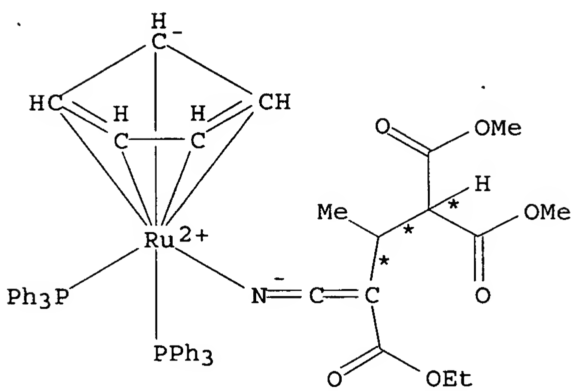
RX(2) OF 8 E + B ===> F



E

B

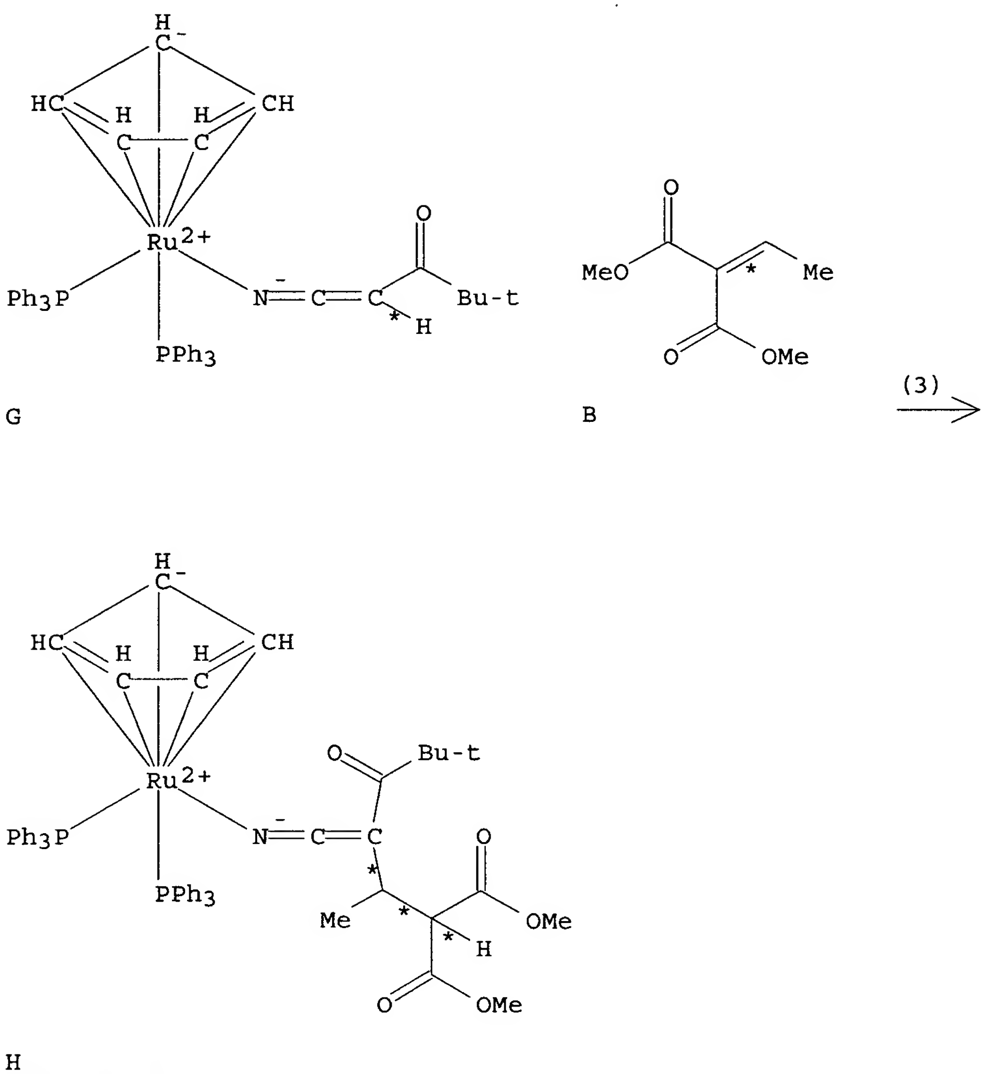
(2)



F
YIELD 98%

RX(2)   RCT E 293767-54-1, B 17041-60-0
         PRO F 330598-55-5
         SOL 71-43-2 Benzene

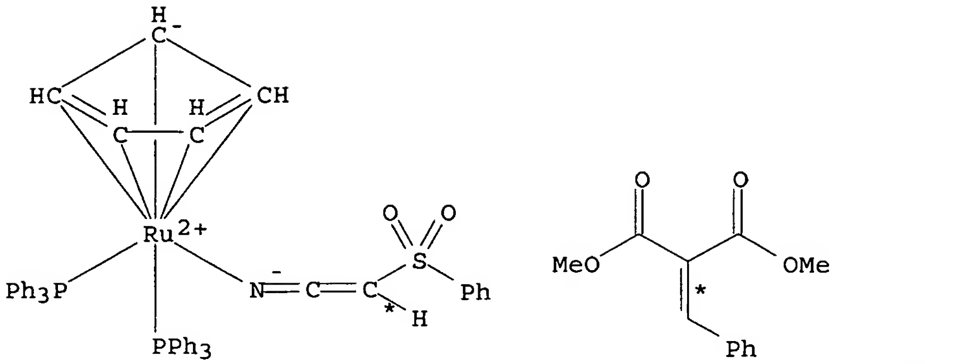
RX(3) OF 8   G + B ===> H



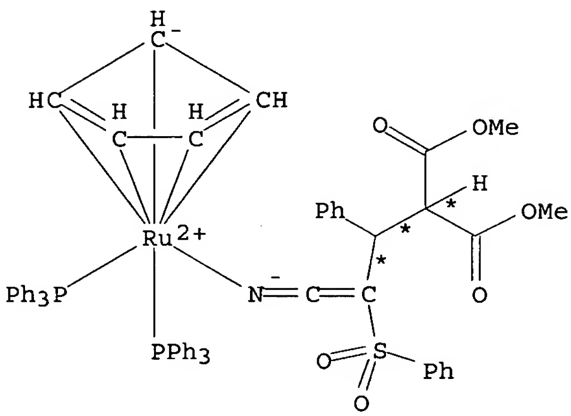
YIELD 98%

RX(3) RCT G **330598-53-3**, B **17041-60-0**
PRO H **330598-56-6**
SOL 71-43-2 Benzene

RX(4) OF 8 A + I ===> J



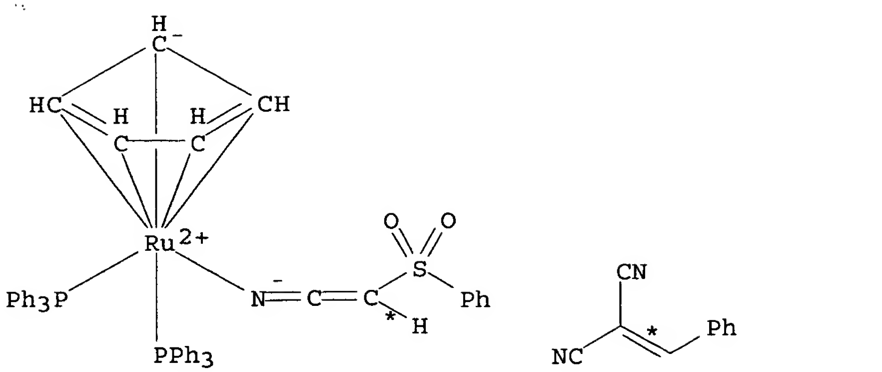
A I



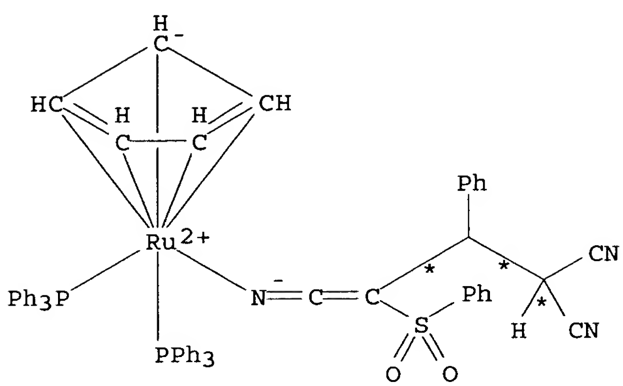
J
YIELD 98%

RX(4) RCT A 264130-83-8, I 6626-84-2
PRO J 330598-57-7
SOL 71-43-2 Benzene

RX(5) OF 8 A + K ===> L



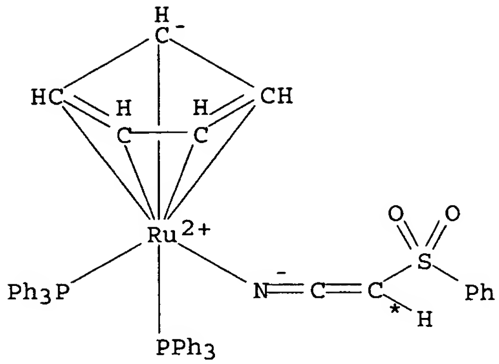
A K



L
YIELD 99%

RX(5) RCT A 264130-83-8, K 2700-22-3
PRO L 330598-58-8
SOL 71-43-2 Benzene

RX(6) OF 8 A + M ===> N



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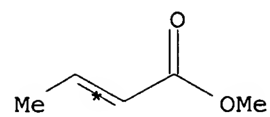
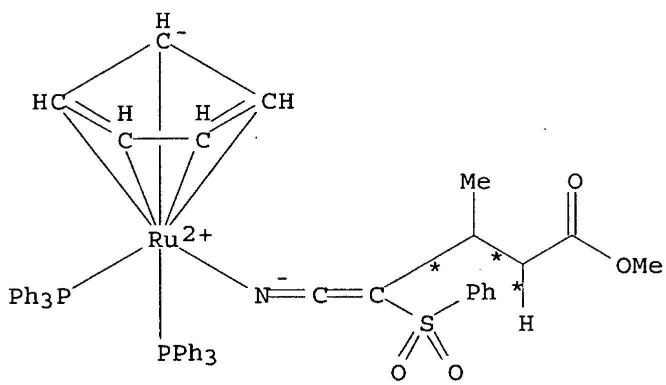


M

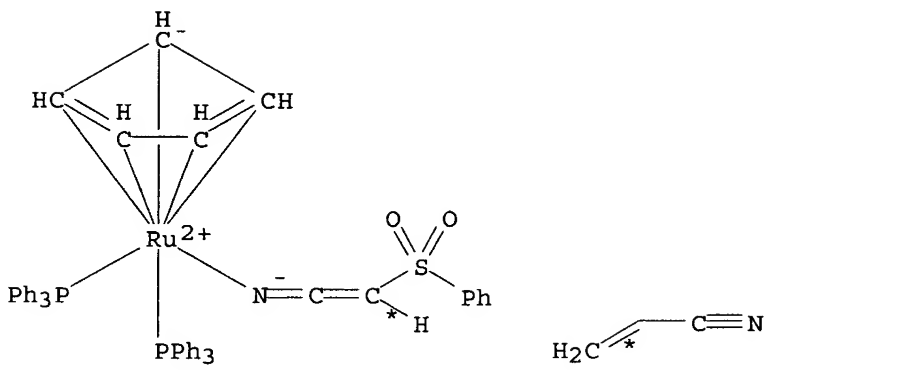
(6) →



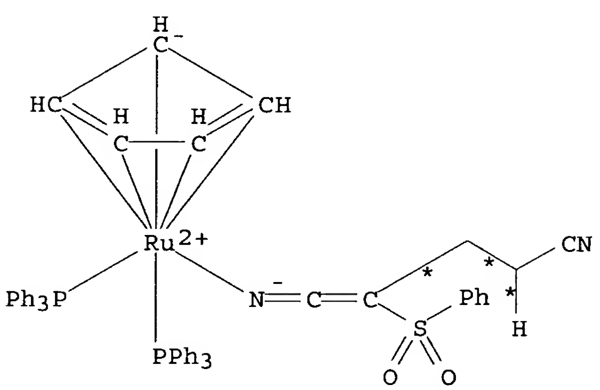
N
YIELD 31%

```
RX(6)       RCT  A 264130-83-8, M 623-43-8
            PRO  N 330598-59-9
            SOL  71-43-2 Benzene
```

```
RX(7) OF 8       A  +  O  ===>  P
```



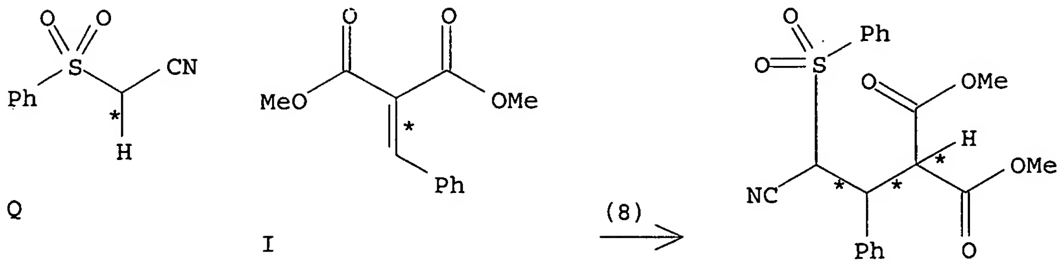
A O



P
YIELD 36%

RX(7) RCT A 264130-83-8, O 107-13-1
PRO P 330598-60-2
SOL 71-43-2 Benzene

RX(8) OF 8 Q + I ===> R

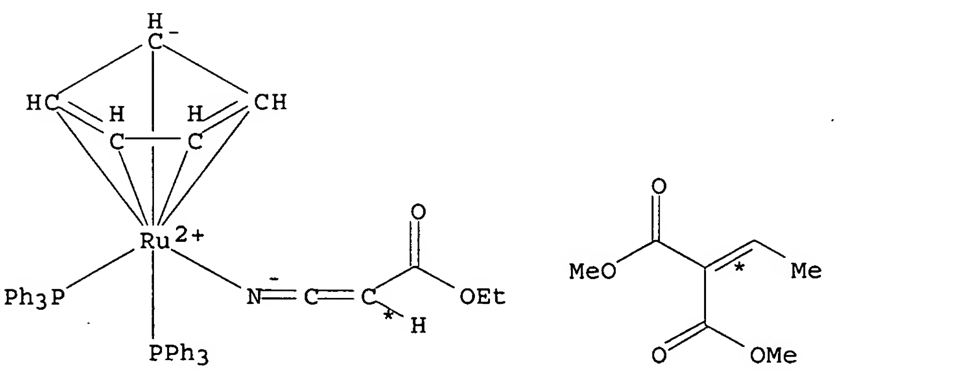


Q I R

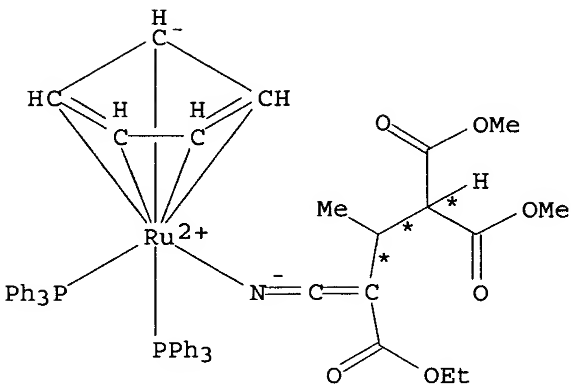
YIELD 88%

RX(8) RCT Q 7605-28-9, I 6626-84-2
PRO R 330598-61-3
CAT 330598-57-7 Ruthenium, (η5-2,4-cyclopentadien-1-yl)[dimethyl [3-(imino-κN)-1-phenyl-2-(phenylsulfonyl)-2-propenyl]propanedioato]bis(triphenylphosphine)-
SOL 109-99-9 THF
NTE Michael addn. reaction

RX(2) OF 8 **E + B ===> F**



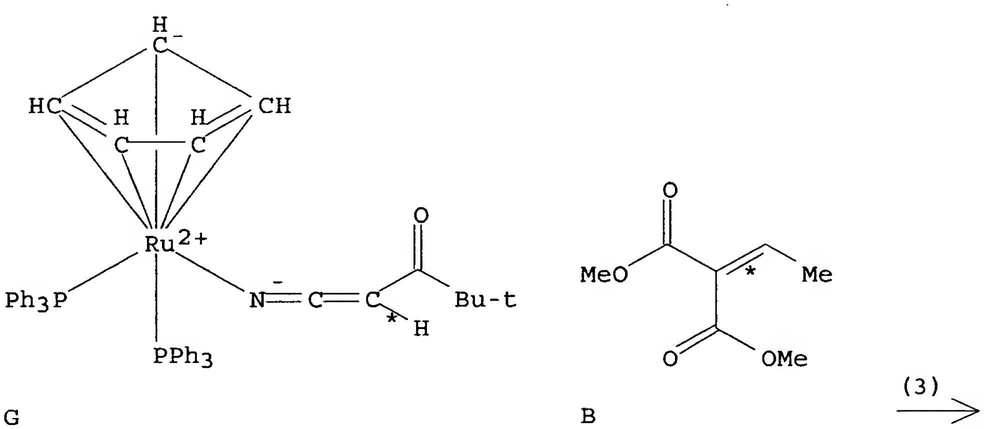
E B



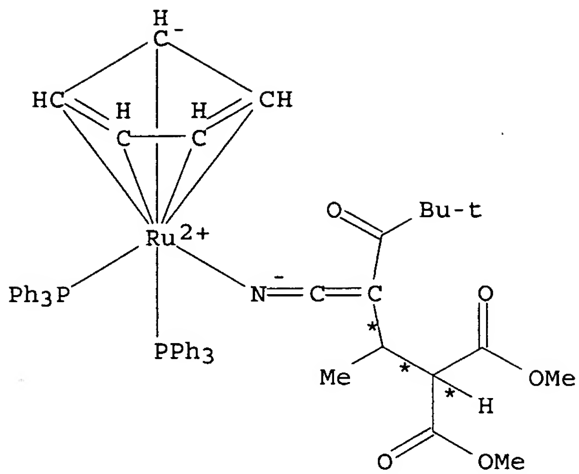
F
YIELD 98%

RX(2) RCT E **293767-54-1**, B **17041-60-0**
PRO F **330598-55-5**
SOL 71-43-2 Benzene

RX(3) OF 8 **G** + **B** ===> **H**



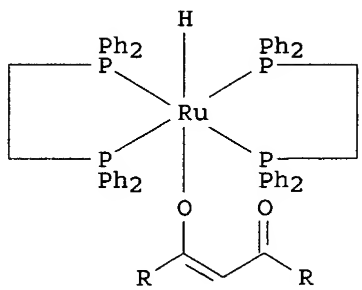
G B



H
YIELD 98%

RX(3)   RCT G **330598-53-3**, B **17041-60-0**
           PRO H **330598-56-6**
           SOL 71-43-2 Benzene

L20 ANSWER 3 OF 7 CASREACT COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 129:175347 CASREACT
TITLE: Michael reactions promoted by η1-O-enolatoruthenium(II) complexes derived from Ru(cod)(cot), diphosphine, and dimethyl malonate
AUTHOR(S): Alvarez, Salvador G.; Hasegawa, Sachi; Hirano, Masafumi; Komiya, Sanshiro
CORPORATE SOURCE: Department of Applied Chemistry, Faculty of Technology, Tokyo University of Agriculture and Technology, Tokyo, 184-8588, Japan
SOURCE: Tetrahedron Letters (1998), 39(29), 5209-5212
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
CLASSIFICATION: 23-17 (Aliphatic Compounds)
Section cross-reference(s): 29
GRAPHIC IMAGE:



I

ABSTRACT:
The Michael reaction of 1,3-dicarbonyls with α,β-unsatd. esters and nitriles has been carried out very efficiently, under mild and neutral conditions, in the presence of a catalytic amount of trans-hydrido(η1-O-enolato) ruthenium(II) complex I. I is prepared from the reaction of Ru(cod)(cot)(cod = cycloocta-1,5-diene; cot = cycloocta-1,3,5-triene) with di-Me malonate in the presence of Ph2P(CH2)2PPh2 (dpe). I catalyzes the Michael reaction of Me acrylate with a 1:1 mixture of di-Me malonate and acetylacetone to give the double Michael adduct of Me acrylate with acetylacetone exclusively in 67% yield; NaOMe in THF provides the double Michael adducts of acetylacetone and di-Me malonate, resp., in a 28:72 ratio, while PEt3 gives the adducts in a ratio of 86:14.

SUPPL. TERM: ruthenium enolato hydride complex catalyst prepn; heptanedioate methoxycarbonyl prepn; acetyl heptanedioate prepn; methoxycarbonyl heptanedinitrile prepn; heptanedinitrile diacetyl prepn; Michael addn reaction catalyst acrylate acrylonitrile; acetylacetone malonate Michael addn catalyst; enolato ruthenium complex catalyst Michael addn; selective Michael addn catalyst proton acidity

INDEX TERM: Chemoselectivity
Michael reaction
Michael reaction catalysts
(η1-enolato ruthenium(2+) complexes as catalysts for the double Michael addition of acetylacetone and di-Me malonate to Me acrylate and acrylonitrile)

INDEX TERM: 211634-64-9P
ROLE: CAT (Catalyst use); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(η1-enolato ruthenium(2+) complexes as catalysts for the double Michael addition of acetylacetone and di-Me malonate to Me acrylate and acrylonitrile)

INDEX TERM: 211634-66-1P
ROLE: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(η1-enolato ruthenium(2+) complexes as catalysts for the double Michael addition of acetylacetone and di-Me malonate to Me acrylate and acrylonitrile)

INDEX TERM: 96-33-3 107-13-1, 2-Propenenitrile, reactions
108-59-8, Dimethyl malonate 123-54-6,

2,4-Pentanedione, reactions 1663-45-2,
1,2-Bis(diphenylphosphino)ethane 42516-72-3
ROLE: RCT (Reactant); RACT (Reactant or reagent)
(η1-enolato ruthenium(2+) complexes as catalysts for the double Michael addition of acetylacetone and di-Me malonate to Me acrylate and acrylonitrile)

INDEX TERM: 609-02-9P 815-57-6P 5324-43-6P 13984-59-3P 19766-36-0P 22711-92-8P 211634-65-0P
ROLE: SPN (Synthetic preparation); PREP (Preparation)
(η1-enolato ruthenium(2+) complexes as catalysts for the double Michael addition of acetylacetone and di-Me malonate to Me acrylate and acrylonitrile)

REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD.

REFERENCE(S):

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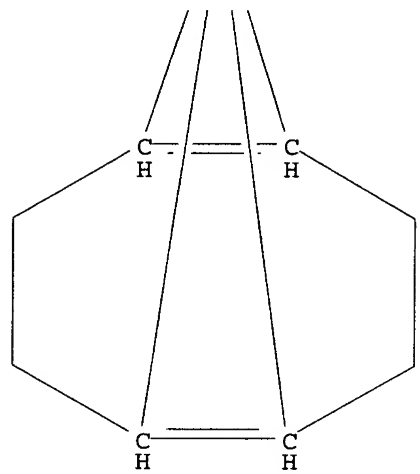
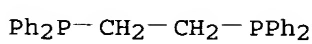
RX(1) OF 12 A + 2 B + C ===> D...

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT
*

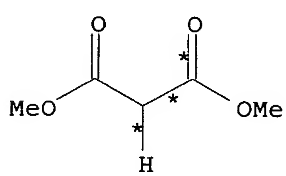
PAGE 2-A



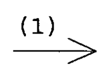
A

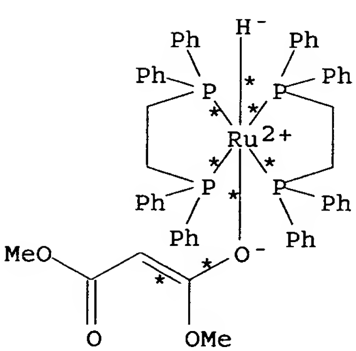


2 B



C





D
YIELD 21%

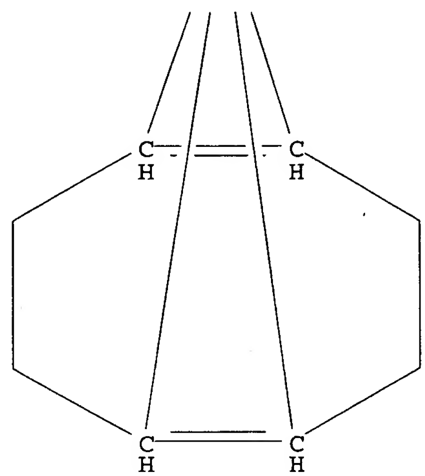
RX(1) RCT A 42516-72-3, B 1663-45-2, C 108-59-8

PRO D 211634-64-9
SOL 71-43-2 Benzene

RX(2) OF 12 A + B + F ===> G

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

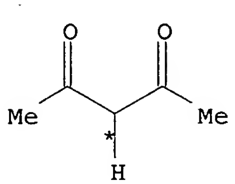
PAGE 2-A



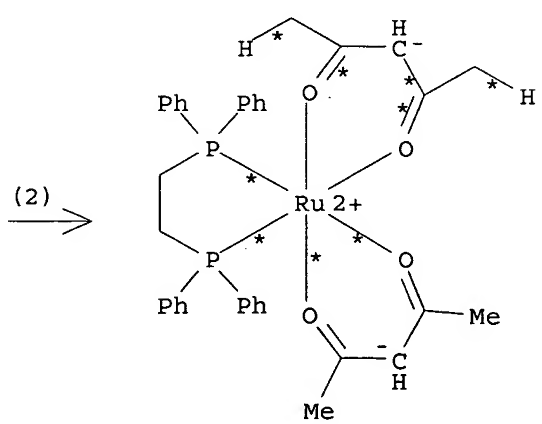
A

$Ph_2P-CH_2-CH_2-PPh_2$

B



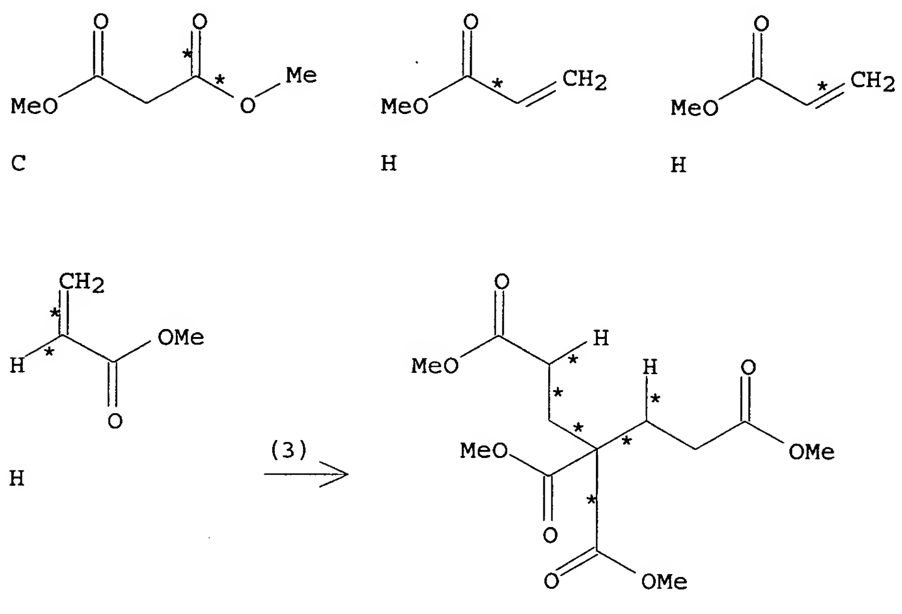
F



G
YIELD 12%

RX(2) RCT A 42516-72-3, B 1663-45-2, F 123-54-6
PRO G 211634-65-0
SOL 71-43-2 Benzene

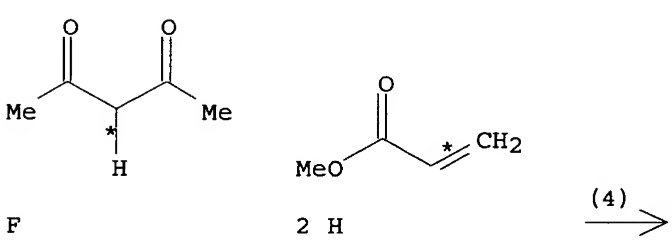
RX(3) OF 12 C + 3 H ===> I

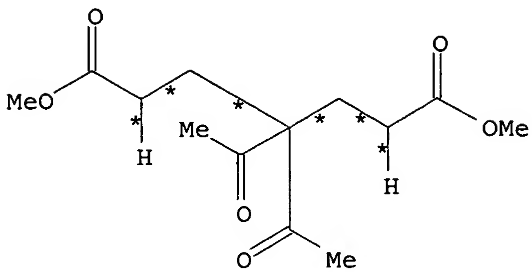


I
YIELD 89%

RX(3) RCT C 108-59-8, H 96-33-3
PRO I 19766-36-0
CAT 211634-66-1 Ruthenium, bis[1,2-ethanediylbis[diphenylphosphine-κP]]hydro[4-(hydroxy-κO)-3-penten-2-onato]-, (OC-6-11)-
SOL 71-43-2 Benzene
NTE chemoselective, yield based on di-Me malonate

RX(4) OF 12 F + 2 H ===> K

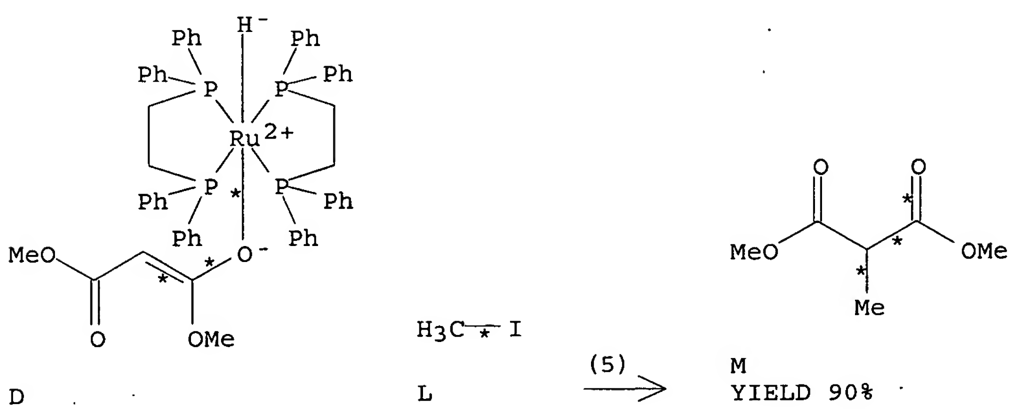




K
YIELD 62%

RX(4)   RCT F 123-54-6, H 96-33-3
         PRO K 13984-59-3
         CAT 211634-66-1 Ruthenium, bis[1,2-ethanediylbis[diphenylphosphine-κP]]hydro[4-(hydroxy-κO)-3-penten-2-onato]-, (OC-6-11)-
         SOL 71-43-2 Benzene
         NTE chemoselective, yield based on 1,3-pentanedione

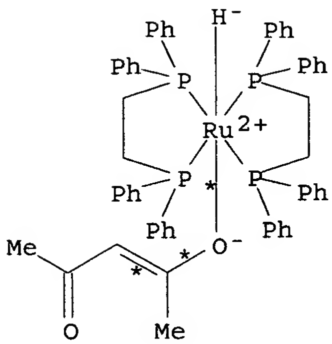
RX(5) OF 12   ...D + L ===> M



D   L   M
YIELD 90%

RX(5)   RCT D 211634-64-9, L 74-88-4
         PRO M 609-02-9
         SOL 1076-43-3 C6D6

RX(6) OF 12   J + L ===> O

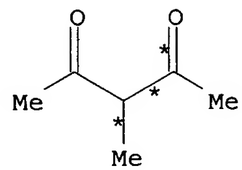


J

H_3C * I

L

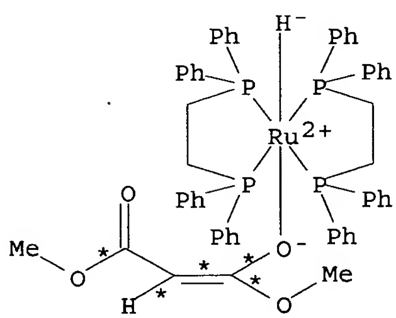
$\xrightarrow{(6)}$



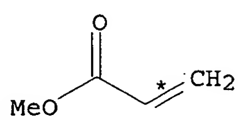
O
YIELD 73%

RX(6) RCT J 211634-66-1, L 74-88-4
PRO O 815-57-6
SOL 1076-43-3 C6D6

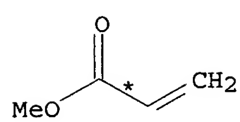
RX(7) OF 12 ...D + 3 H ===> I



D

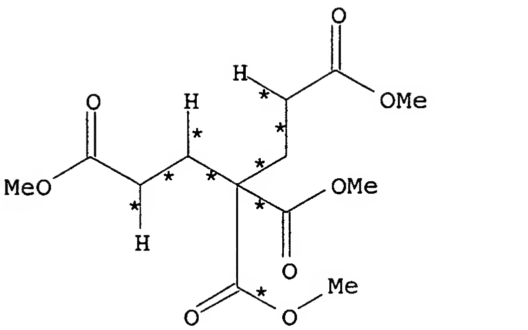


2 H



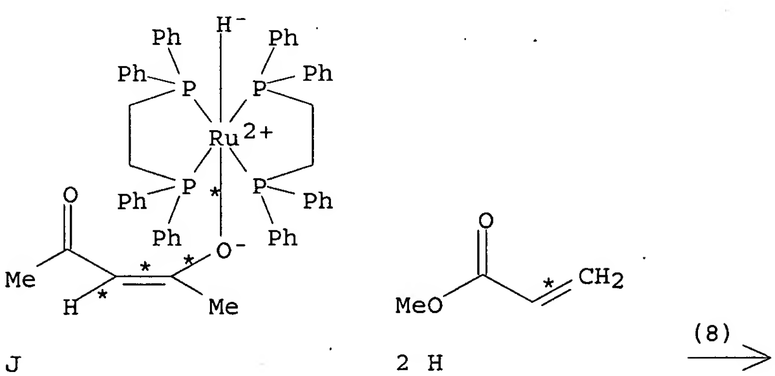
H

$\xrightarrow{(7)}$

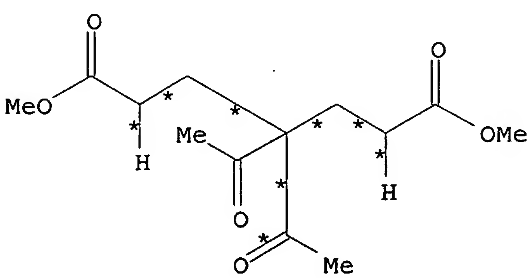


I
YIELD 89%

```
RX(7)      RCT  D 211634-64-9, H 96-33-3
           PRO  I 19766-36-0
           SOL  1076-43-3 C6D6

RX(8) OF 12      J  +  2 H  ===>  K
```



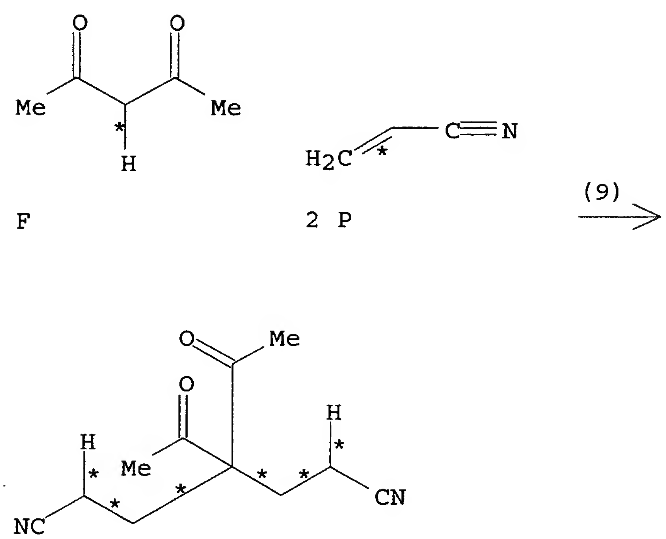
J 2 H



K
YIELD 91%

RX(8) RCT J 211634-66-1, H 96-33-3
PRO K 13984-59-3
SOL 1076-43-3 C6D6

RX(9) OF 12 F + 2 P ===> Q

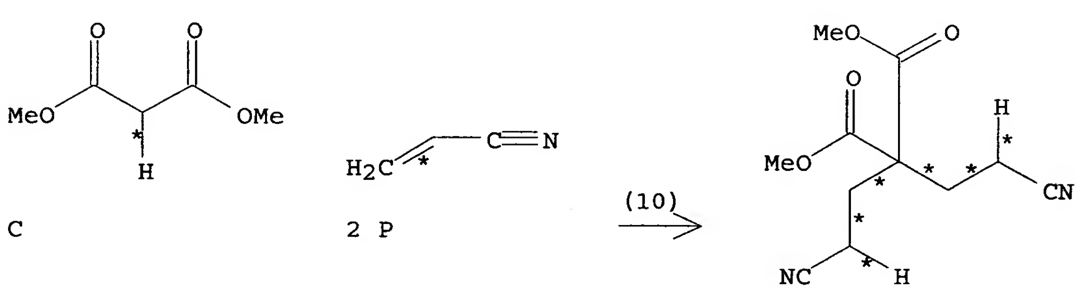


F 2 P

Q
YIELD 70%

RX(9) RCT F 123-54-6, P 107-13-1
PRO Q 5324-43-6
CAT 211634-64-9 Ruthenium, bis[1,2-ethanediylbis[diphenylphosphine-κP]]hydro[methyl 3-(hydroxy-κO)-3-methoxy-2-propenoato]-, (OC-6-11)-
SOL 71-43-2 Benzene
NTE chemoselective, yield based on 1,3-pentanedione

RX(10) OF 12 C + 2 P ===> R



C 2 P

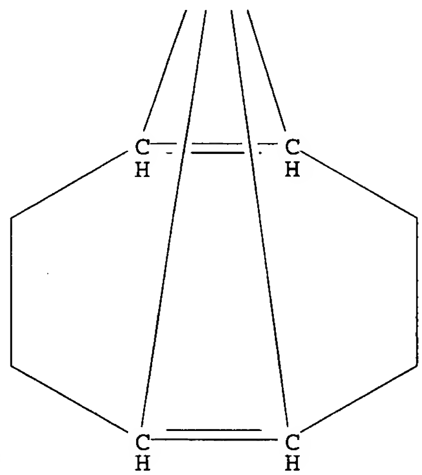
R
YIELD 24%

RX(10) RCT C 108-59-8, P 107-13-1
PRO R 22711-92-8
CAT 211634-64-9 Ruthenium, bis[1,2-ethanediylbis[diphenylphosphine-κP]]hydro[methyl 3-(hydroxy-κO)-3-methoxy-2-propenoato]-, (OC-6-11)-
SOL 71-43-2 Benzene
NTE chemoselective, yield based on di-Me malonate

RX(12) OF 12 COMPOSED OF RX(1), RX(7)
RX(12) **A** + 2 B + **C** + 3 **H** ===>
I

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT
*

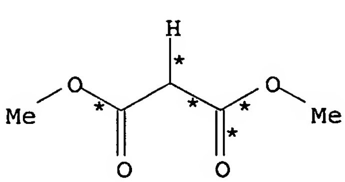
PAGE 2-A



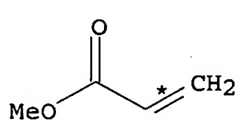
A

$Ph_2P—CH_2—CH_2—PPh_2$

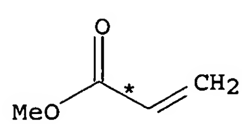
2 B



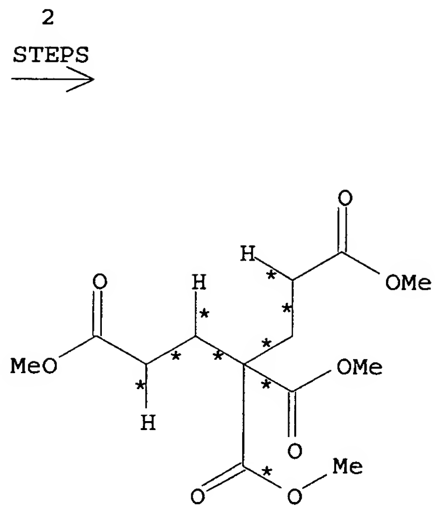
C



2 H



H



I
YIELD 89%

RX(1) RCT A **42516-72-3**, B 1663-45-2, C **108-59-8**
PRO D 211634-64-9
SOL 71-43-2 Benzene

RX(7) RCT D 211634-64-9, H **96-33-3**
PRO I **19766-36-0**
SOL 1076-43-3 C6D6

L20 ANSWER 4 OF 7 CASREACT COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 118:255103 CASREACT
TITLE: Synthesis of 2-transition-metal-substituted 1,3-butadienyl complexes with unusual structures and facile Diels-Alder reactions of cobalt 1,3-butadiene complexes
AUTHOR(S): Smalley, Terrence L., Jr.; Wright, Marcus W.; Garmon, Stuart A.; Welker, Mark E.; Rheingold, Arnold L.
CORPORATE SOURCE: Dep. Chem., Wake Forest Univ., Winston-Salem, NC, 27109, USA
SOURCE: Organometallics (1993), 12(4), 998-1000
CODEN: ORGND7; ISSN: 0276-7333
DOCUMENT TYPE: Journal
LANGUAGE: English
CLASSIFICATION: 29-13 (Organometallic and Organometalloidal Compounds)
Section cross-reference(s): 24

ABSTRACT:
The cyclopentadienyliron dicarbonyl anion and (Rpy)(DMG)2Co anions (DMG = dimethylglyoximato; R = H, t-Bu) react cleanly with 1,2-butadienyl chlorides and tosylates to generate transition-metal-substituted 1,3-butadienes CH2:C(MLn)CH:CH2 [MLn = CpFe(CO)2, (py)(DMG)2Co, (4-t-Bupy)(DMG)2Co]. The cobalt-substituted 1,3-butadienes react under mild conditions and with high regioselectivity with a variety of dienophiles to yield transition-metal-substituted cyclohexenes. A

variety of cyclohexanoid products can subsequently be obtained from these transition-metal-substituted cyclohexenes via demetalation reactions.

SUPPL. TERM: Diels Alder cobalt butadiene complex; transition metal substituted butadienyl complex; cyclohexene deriv organometallic prepn

INDEX TERM: Regiochemistry
(of Diels-Alder reaction of cobalt butadiene complexes)

INDEX TERM: Diels-Alder reaction
Kinetics of Diels-Alder reaction
(of cobalt butadiene complexes)

INDEX TERM: 80-62-6, Methyl methacrylate 96-33-3, Methyl acrylate 97-63-2, Ethyl methacrylate 106-51-4, 2,5-Cyclohexadiene-1,4-dione, reactions 108-31-6, Maleic anhydride, reactions 140-88-5, Ethyl acrylate 624-48-6, Dimethyl maleate 624-49-7, Dimethyl fumarate 762-21-0, Diethyl acetylene dicarboxylate 3377-20-6 3377-21-7, Dimethyl methylene malonate
ROLE: RCT (Reactant); RACT (Reactant or reagent)
(Diels-Alder reaction of, with cobalt-substituted butadiene)

INDEX TERM: 142617-67-2P 147735-85-1P
ROLE: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and Diels-Alder reactions of)

INDEX TERM: 147735-88-4P
ROLE: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and demetalation of)

INDEX TERM: 25790-55-0P 147396-58-5P
ROLE: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, with transition metal anions)

INDEX TERM: 38511-09-0P 55704-60-4P 60372-92-1P
142617-59-2P 142617-60-5P 142808-86-4P
147396-57-4P 147583-82-2P 147583-83-3P
147583-84-4P 147735-86-2P 147735-87-3P
147735-89-5P 147735-90-8P 147735-91-9P
147762-44-5P 147782-96-5P 147782-97-6P
147782-98-7P
ROLE: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

INDEX TERM: 12152-20-4 75699-52-4 130351-49-4
ROLE: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with butadienyl chloride or tosylate)

INDEX TERM: 110-86-1, Pyridine, reactions 3978-81-2
ROLE: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with cobalt chloride hexahydrate and dimethylglyoxime)

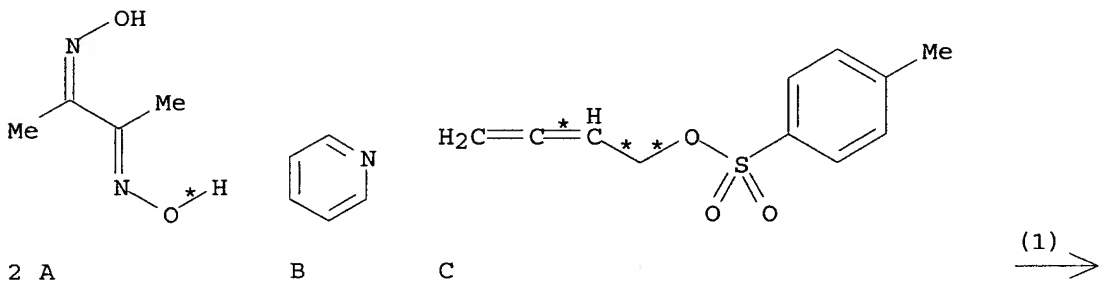
INDEX TERM: 95-45-4, Dimethylglyoxime
ROLE: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with cobalt chloride hexahydrate and pyridines)

INDEX TERM: 7791-13-1 13815-10-6

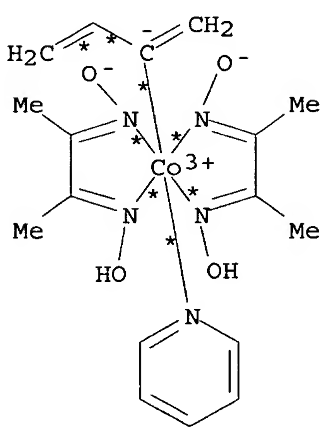
ROLE: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with dimethylglyoxime and
pyridines)

INDEX TERM: 18913-31-0, 2,3-Butadien-1-ol
ROLE: RCT (Reactant); RACT (Reactant or reagent)
(reactions of)

RX(1) OF 23 2 A + B + C ===> D...



2 A B C



D
YIELD 75%

RX(1) RCT A 95-45-4

STAGE(1)
RGT E 13815-10-6 Cobalt(2+), hexaaqua-, dichloride,
(OC-6-11)-
SOL 67-56-1 MeOH

STAGE(2)
RCT B 110-86-1
RGT F 75-09-2 CH2Cl2
SOL 7732-18-5 Water

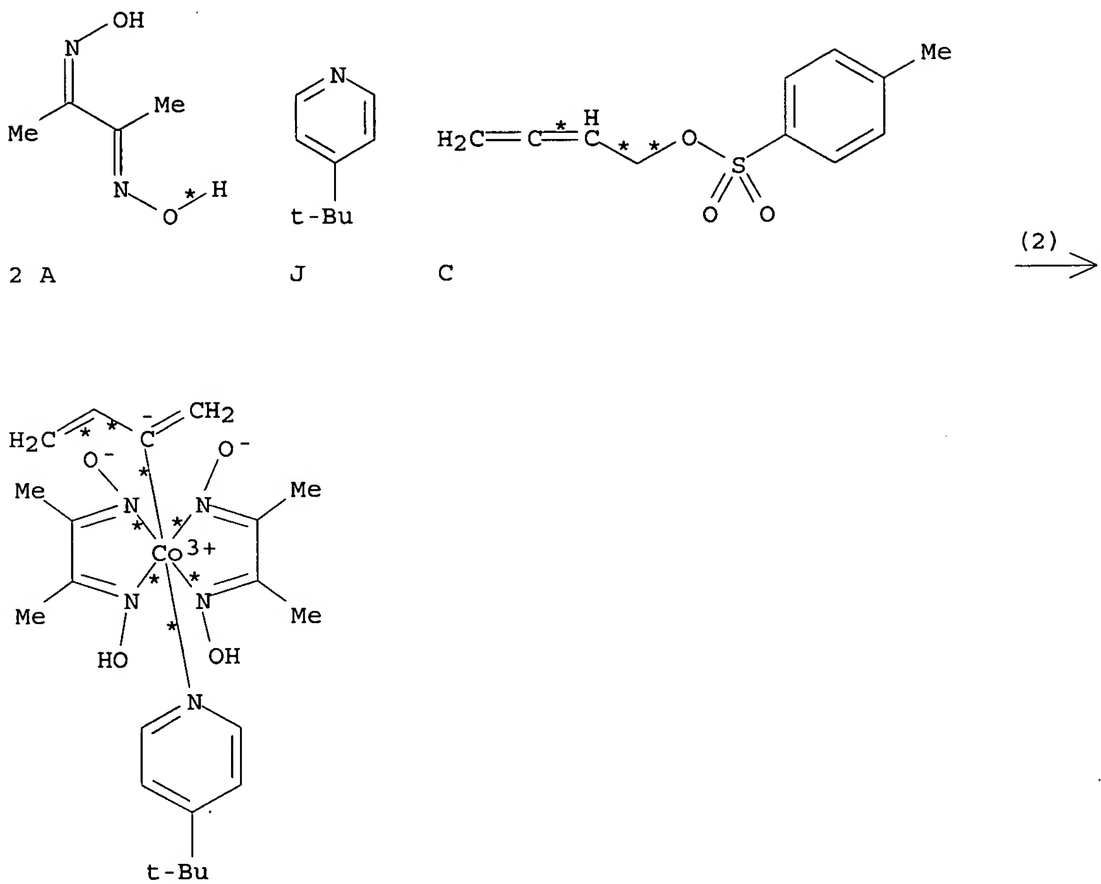
STAGE(3)
RGT G 16940-66-2 NaBH4

SOL 7732-18-5 Water

STAGE(4)
RCT C 147396-58-5

PRO D 142617-67-2

RX(2) OF 23 2 A + J + C ===> K...



K
YIELD 58%

RX(2) RCT A 95-45-4

STAGE(1)
RGT E 13815-10-6 Cobalt(2+), hexaaqua-, dichloride, (OC-6-11)-
SOL 67-56-1 MeOH

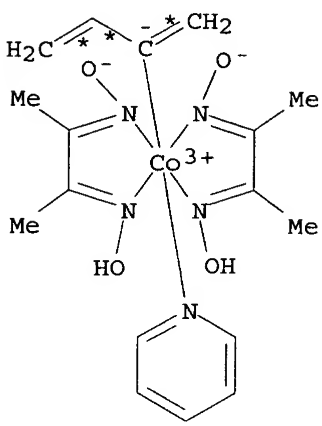
STAGE(2)
RCT J 3978-81-2
RGT F 75-09-2 CH2Cl2
SOL 7732-18-5 Water

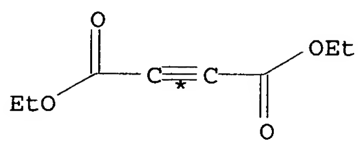
STAGE(3)

RCT C 147396-58-5
RGT G 16940-66-2 NaBH4
SOL 7732-18-5 Water

PRO K 147735-85-1

RX(3) OF 23 ...D + L ===> M



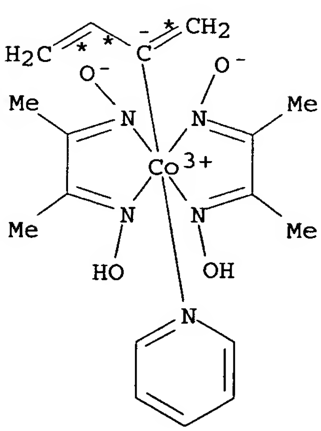


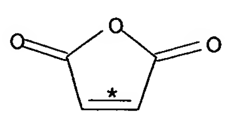
D L (3) →

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

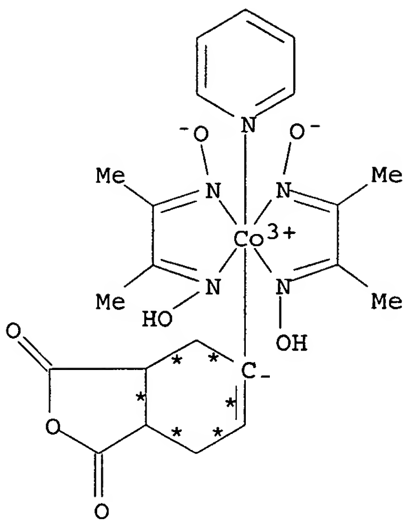
RX(3) RCT D 142617-67-2, L 762-21-0
PRO M 147735-86-2
SOL 109-99-9 THF

RX(4) OF 23 ...D + O ===> P





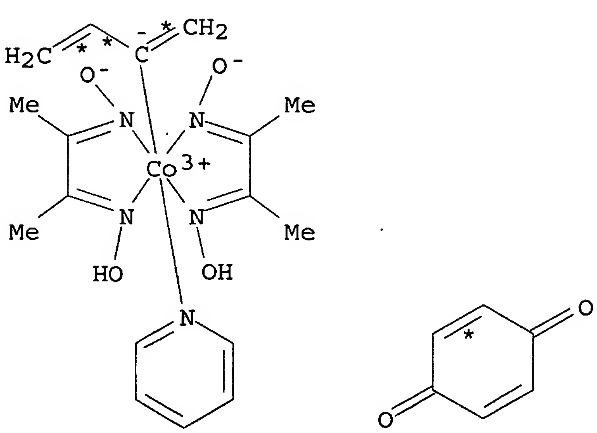
D O (4) →



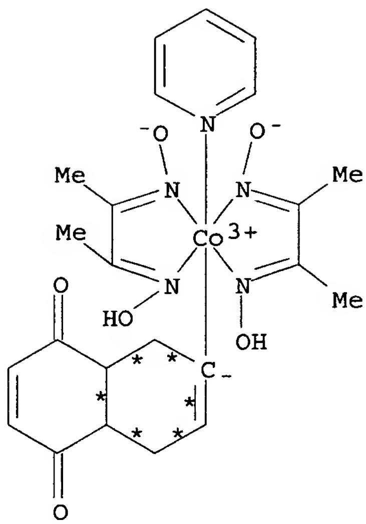
P
YIELD 80%

RX(4)   RCT D 142617-67-2, O 108-31-6
             PRO P 147782-96-5
             SOL 109-99-9 THF

RX(5) OF 23   ...D + Q ===> R



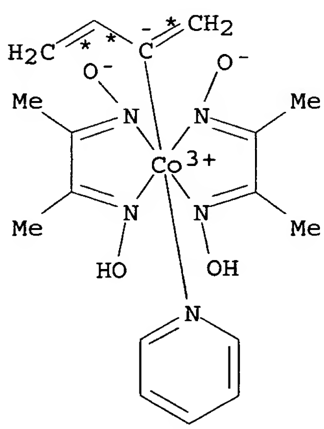
D   Q   (5) →



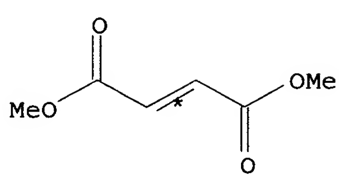
R
YIELD 99%

RX(5) RCT D 142617-67-2, Q 106-51-4
PRO R 147782-97-6
SOL 109-99-9 THF

RX(6) OF 23 ...D + S ===> T



D



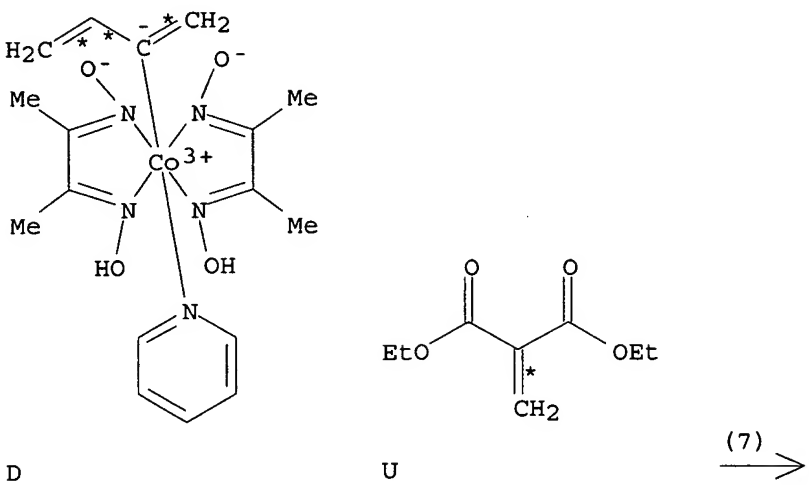
S

(6) →

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT
*

RX(6) RCT D 142617-67-2, S 624-49-7
PRO T 142808-86-4
SOL 109-99-9 THF

RX(7) OF 23 ...D + U ===> V...

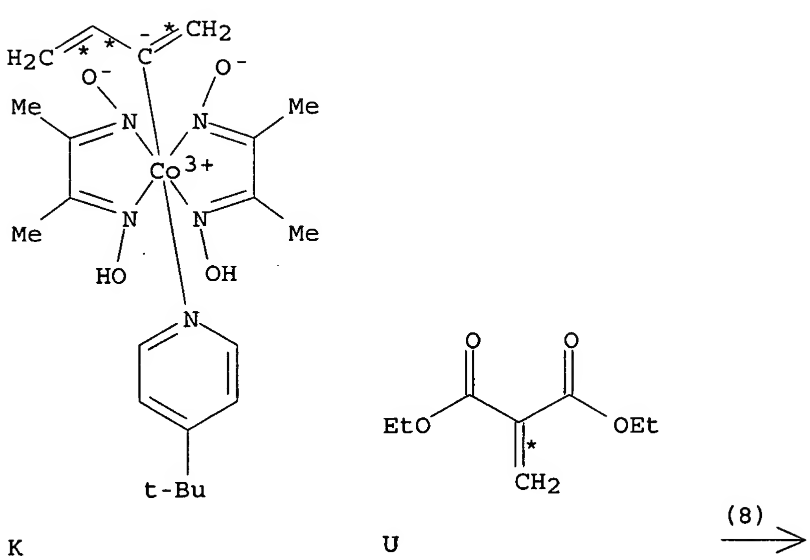


D U (7)

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT
*

RX(7) RCT D 142617-67-2, U 3377-20-6
PRO V 147735-88-4
SOL 109-99-9 THF

RX(8) OF 23 ...K + U ===> W

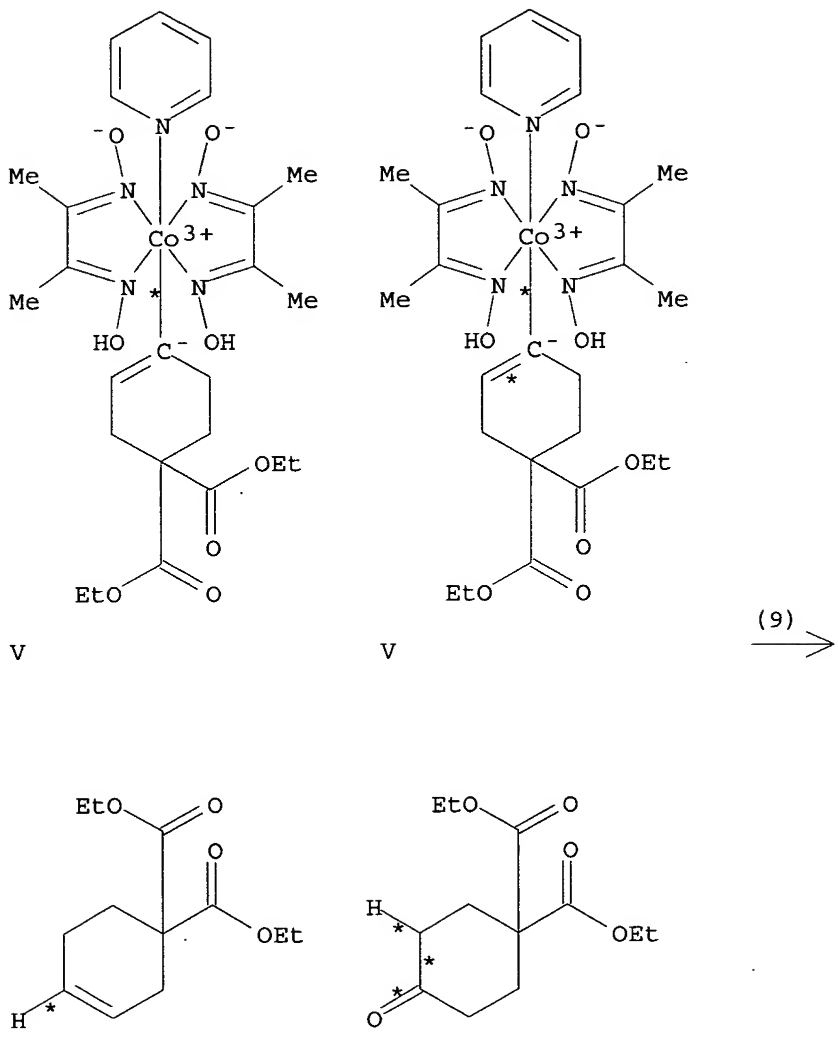


K U (8)

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT
*

RX(8) RCT K 147735-85-1, U 3377-20-6
PRO W 147735-89-5
SOL 109-99-9 THF

RX(9) OF 23 ...2 V ===> X + Y



X
YIELD 42%

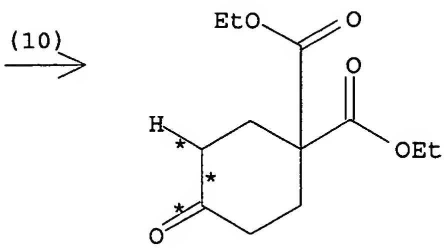
Y
YIELD 34%

RX(9) RCT V 147735-88-4
RGT Z 7647-01-0 HCl
PRO X 38511-09-0, Y 55704-60-4
SOL 75-09-2 CH2Cl2, 7732-18-5 Water

RX(10) OF 23 ...V ===> Y

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT
 *

(10)

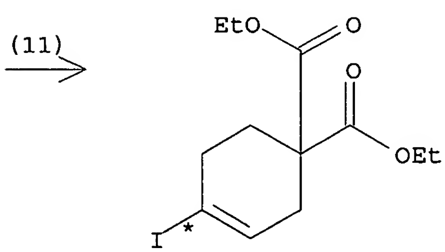


Y
YIELD 48%

```
RX(10)     RCT   V 147735-88-4
           RGT   Z 7647-01-0 HCl, AA 7722-84-1 H2O2
           PRO   Y 55704-60-4
           SOL   75-09-2 CH2Cl2, 7732-18-5 Water

RX(11) OF 23     ...V   ===>   AB
```

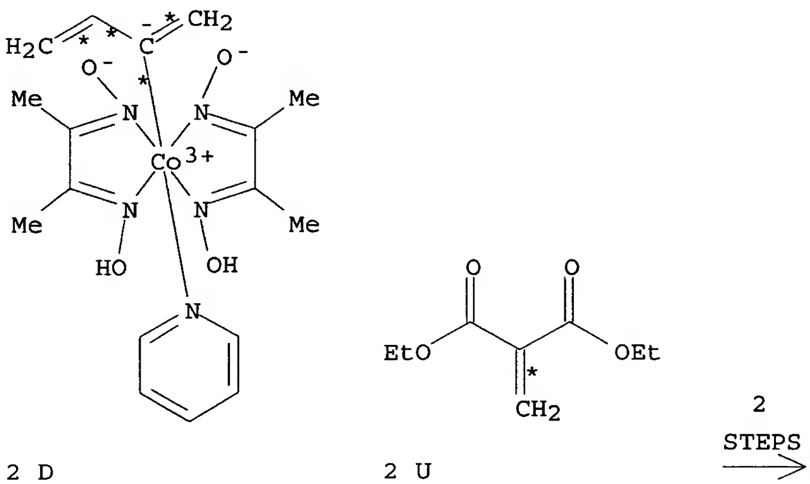
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT
 *

(11)

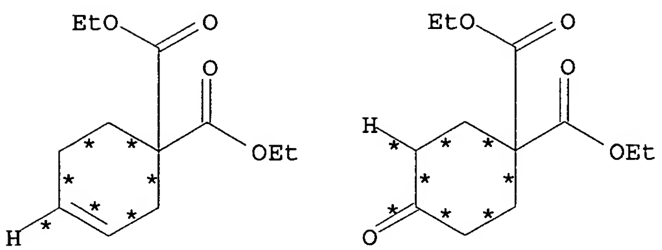


AB
YIELD 76%

```
RX(11)     RCT   V 147735-88-4
           RGT   AC 7553-56-2 I2
           PRO   AB 147396-57-4
           SOL   75-09-2 CH2Cl2

RX(18) OF 23 COMPOSED OF RX(7), RX(9)
RX(18)     2 D  +  2 U   ===>   X  +  Y
```



2 D 2 U

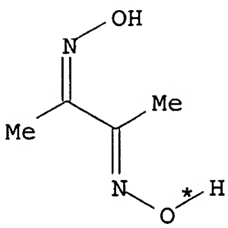


X
YIELD 42%

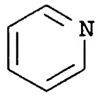
Y
YIELD 34%

RX(7)	RCT	D **142617-67-2**, U **3377-20-6**
	PRO	V 147735-88-4
	SOL	109-99-9 THF
RX(9)	RCT	V 147735-88-4
	RGT	Z 7647-01-0 HCl
	PRO	X 38511-09-0, Y **55704-60-4**
	SOL	75-09-2 CH2Cl2, 7732-18-5 Water

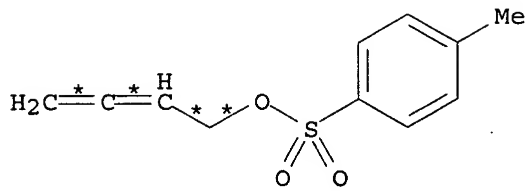
RX(21) OF 23 COMPOSED OF RX(1), RX(7), RX(9)
RX(21) 4 A + 2 B + 2 C + 2 **U** ===> X + **Y**



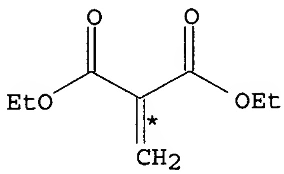
4 A



2 B

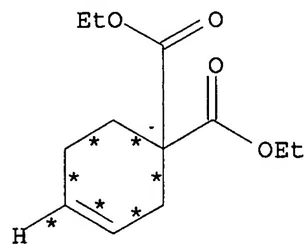


2 C

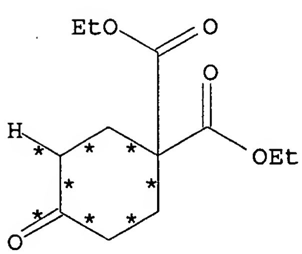


2 U

3
STEPS
→



X
YIELD 42%



Y
YIELD 34%

```
RX(1)     RCT  A 95-45-4

            STAGE(1)
               RGT  E 13815-10-6 Cobalt(2+), hexaaqua-,
                    dichloride, (OC-6-11)-
               SOL  67-56-1 MeOH

            STAGE(2)
               RCT  B 110-86-1
               RGT  F 75-09-2 CH2Cl2
               SOL  7732-18-5 Water

            STAGE(3)
               RGT  G 16940-66-2 NaBH4
               SOL  7732-18-5 Water
```

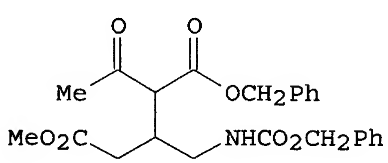
STAGE(4)
RCT C 147396-58-5

PRO D 142617-67-2

RX(7) RCT D 142617-67-2, U **3377-20-6**
PRO V 147735-88-4
SOL 109-99-9 THF

RX(9) RCT V 147735-88-4
RGT Z 7647-01-0 HCl
PRO X 38511-09-0, Y **55704-60-4**
SOL 75-09-2 CH2Cl2, 7732-18-5 Water

L20 ANSWER 5 OF 7 CASREACT COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 111:195366 CASREACT
TITLE: Palladium(II)-assisted carboacylation of enamides to produce functionalized β-amino acids. Synthesis of relays to (±)-thienamycin
AUTHOR(S): Wieber, Gary M.; Hegedus, Louis S.; Akermark, Bjorn; Michalson, Erik T.
CORPORATE SOURCE: Dep. Chem., Colorado State Univ., Fort Collins, CO, 80523, USA
SOURCE: Journal of Organic Chemistry (1989), 54(19), 4649-53
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
CLASSIFICATION: 34-2 (Amino Acids, Peptides, and Proteins)
Section cross-reference(s): 26
GRAPHIC IMAGE:



I

ABSTRACT:
Alkylation of benzyl vinylcarbamate with sodium benzyl acetoacetate in the presence of palladium(II) chloride, followed by carbonylation (CO/MeOH), produced a highly functionalized β-amido ester I, which was converted, using conventional organic synthetic methodol., into a relay to (±)-thienamycin.

SUPPL. TERM: palladium carboacylation enamide; beta amino acid functionalized; thienamycin relay; lactam beta
INDEX TERM: Acylation
(of enamides in presence of palladium, functionalized β-amino acids from)
INDEX TERM: Amides, reactions
ROLE: RCT (Reactant); RACT (Reactant or reagent)
(unsatd., palladium-assisted carboacylation of,

functionalized β-amino acids from)
INDEX TERM: Amino acids, preparation
ROLE: SPN (Synthetic preparation); PREP (Preparation)
(β-, preparation of, by palladium-assisted carboacylation of enamides)
INDEX TERM: Lactams
ROLE: SPN (Synthetic preparation); PREP (Preparation)
(β-, preparation of, palladium-assisted carboacylation of enamides to produce functionalized β-amino acids in relation to)
INDEX TERM: 122313-67-1
ROLE: RCT (Reactant); RACT (Reactant or reagent)
(alkylation by, of benzyl vinylcarbamate in presence of palladium chloride)
INDEX TERM: 7440-05-3, Palladium, uses and miscellaneous
ROLE: USES (Uses)
(carboacylation of enamides in presence of, functionalized β-amino acids from)
INDEX TERM: 84713-20-2P
ROLE: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and alkylation of, with sodium benzyl acetoacetate in presence of palladium chloride, carbonylation of product from)
INDEX TERM: 122313-57-9P 122313-59-1P 122313-60-4P
ROLE: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and cyclocondensation of, β-lactam from)
INDEX TERM: 122313-64-8P 122313-65-9P
ROLE: SPN (Synthetic preparation); PREP (Preparation)
(preparation and deketalization)
INDEX TERM: 122313-61-5P 122313-62-6P
ROLE: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and deketalization or silylation of)
INDEX TERM: 122313-55-7P 122313-56-8P
ROLE: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and hydride reduction of)
INDEX TERM: 122313-69-3P 122313-70-6P 122313-71-7P
ROLE: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and hydrogenolysis of)
INDEX TERM: 50830-56-3P, Acryloyl azide
ROLE: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, with benzyl alc.)
INDEX TERM: 122313-63-7P 122332-75-6P
ROLE: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reduction of)
INDEX TERM: 86421-11-6P 106248-39-9P 122313-68-2P
ROLE: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and O-silylation of, with tert-butyldimethylsilyl chloride)

INDEX TERM: 86421-12-7P 93711-82-1P 122313-53-5P
122313-54-6P 122313-66-0P 122405-37-2P
136353-97-4P
ROLE: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

INDEX TERM: 65750-57-4
ROLE: RCT (Reactant); RACT (Reactant or reagent)
(preparation of relays to, palladium-assisted carboacylation of enamides to produce functionalized β-amino acids in relation to)

INDEX TERM: 100-51-6, Benzenemethanol, reactions
ROLE: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with acryloyl azide)

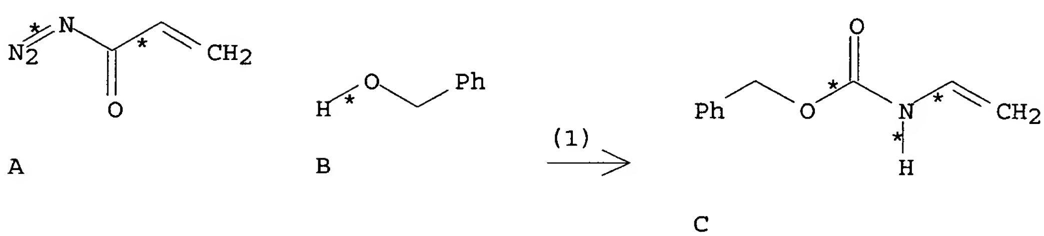
INDEX TERM: 814-68-6, 2-Propenoyl chloride
ROLE: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with azide)

INDEX TERM: 609-08-5, Diethyl methylmalonate
ROLE: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with benzyl vinylcarbamate palladium complex)

INDEX TERM: 69739-34-0, tert-Butyldimethylsilyl triflate
ROLE: RCT (Reactant); RACT (Reactant or reagent)
(N-silylation by, of β-lactam)

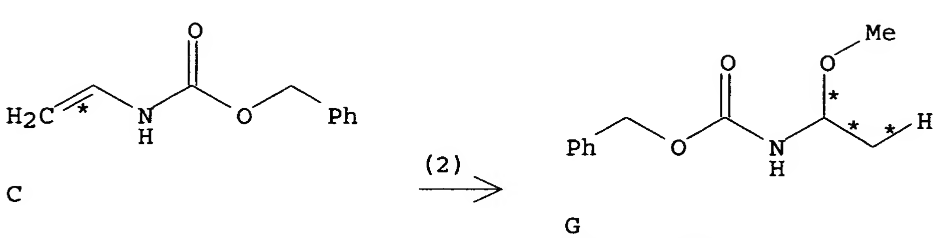
INDEX TERM: 18162-48-6, tert-Butyldimethylsilyl chloride
ROLE: RCT (Reactant); RACT (Reactant or reagent)
(O-silylation by, of hydroxyhexanoic acid derivative)

RX(1) OF 100 ...A + B ===> C...



RX(1) RCT A 50830-56-3, B 100-51-6
RGT D 123-31-9 Hydroquinone, E 110-86-1 Pyridine
PRO C 84713-20-2
SOL 108-88-3 PhMe

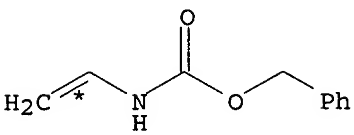
RX(2) OF 100 ...C ===> G



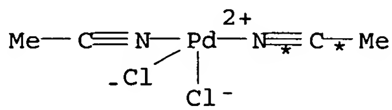
YIELD 76%

RX(2) RCT C 84713-20-2
RGT H 14592-56-4 PdCl2(MeCN)2, I 121-44-8 Et3N, J 1333-74-0 H2, K 67-56-1 MeOH
PRO G 136353-97-4
SOL 67-56-1 MeOH

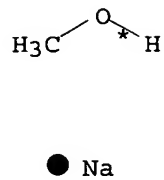
RX(3) OF 100 ...C + H + L ===> M



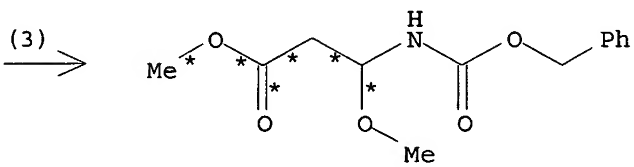
C



H



L



M
YIELD 67%

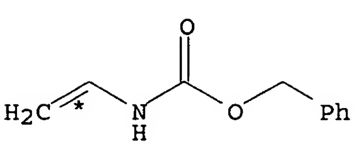
RX(3) RCT C 84713-20-2, H 14592-56-4

STAGE(1)
SOL 109-99-9 THF

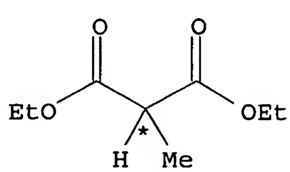
STAGE(2)
RCT L 124-41-4
RGT I 121-44-8 Et3N
SOL 109-99-9 THF

PRO M 122313-53-5

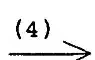
RX(4) OF 100 ...C + O ===> P

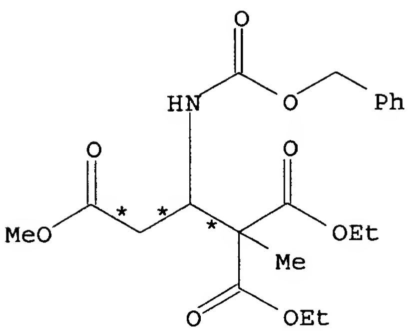


C



O





P
YIELD 63%

RX(4) RCT C 84713-20-2

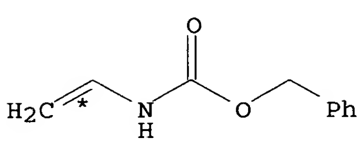
STAGE(1)
RGT H 14592-56-4 PdCl2(MeCN)2
SOL 109-99-9 THF

STAGE(2)
RCT O 609-08-5
RGT Q 16940-66-2 NaBH4
SOL 109-99-9 THF

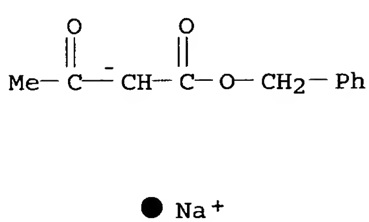
STAGE(3)
RGT I 121-44-8 Et3N
SOL 109-99-9 THF

PRO P 122313-54-6

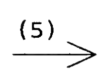
RX(5) OF 100 ...2 C + 2 R ===> S + T...

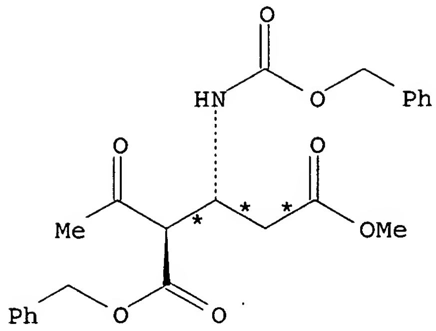


2 C

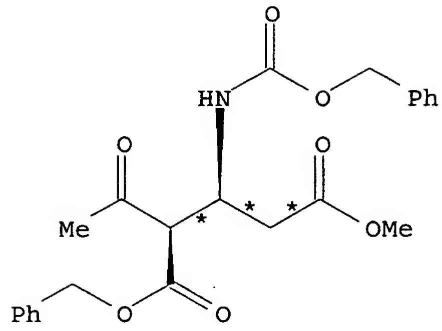


2 R





S
YIELD 92%(50)



T
YIELD 92%(50)

RX(5) RCT C 84713-20-2

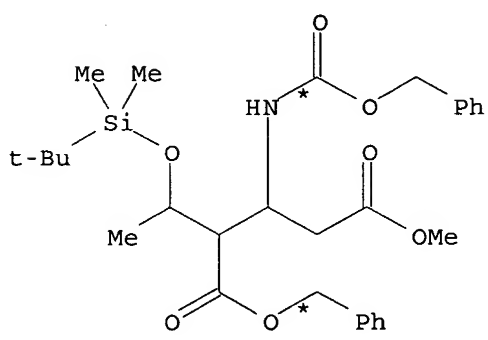
STAGE(1)
RGT H 14592-56-4 PdCl2(MeCN)2, I 121-44-8 Et3N
SOL 109-99-9 THF

STAGE(2)
RCT R 122313-67-1
SOL 109-99-9 THF

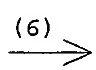
STAGE(3)
RGT K 67-56-1 MeOH, U 630-08-0 CO
SOL 109-99-9 THF, 67-56-1 MeOH

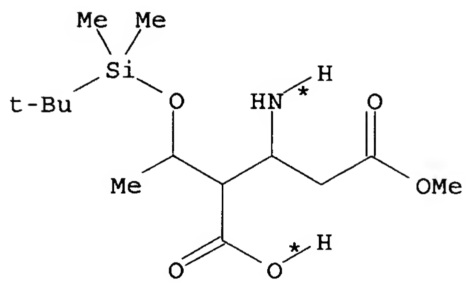
PRO S 122313-55-7, T 122313-56-8

RX(6) OF 100 ...V ===> W...



V

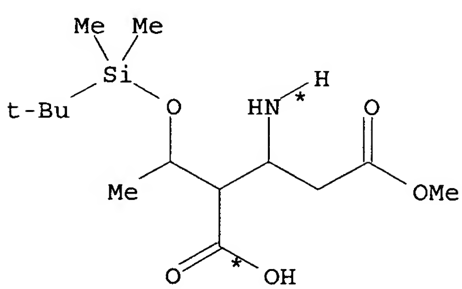




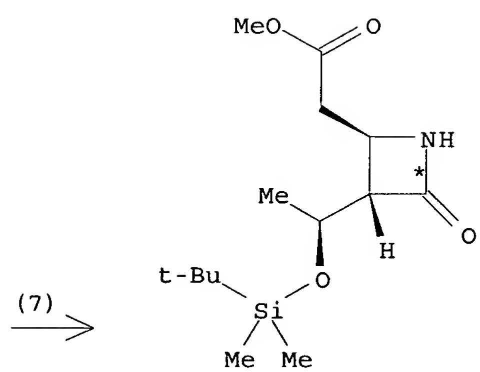
W
YIELD 95%

RX(6)	RCT	V 122313-69-3
	RGT	J 1333-74-0 H2
	PRO	W 122313-57-9
	CAT	7440-05-3 Pd
	SOL	67-56-1 MeOH

RX(7) OF 100 ...W ===> Y



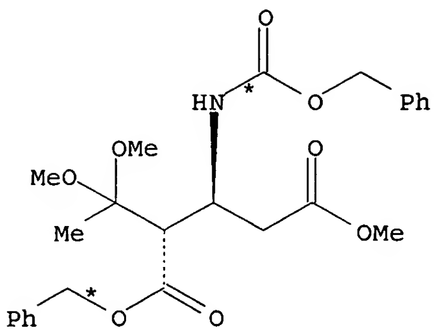
W



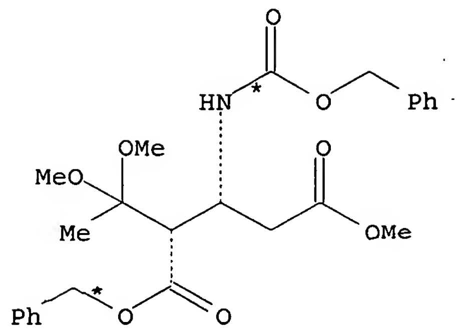
Y
YIELD 95%

RX(7)	RCT	W 122313-57-9
	RGT	Z 538-75-0 DCC
	PRO	Y 86421-12-7
	SOL	109-99-9 THF

RX(8) OF 100 ...AA + AB ===> AC + AD...

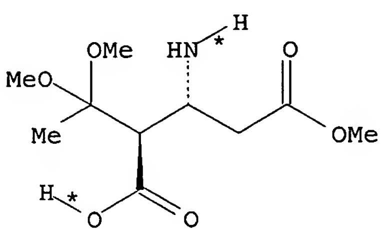


AA

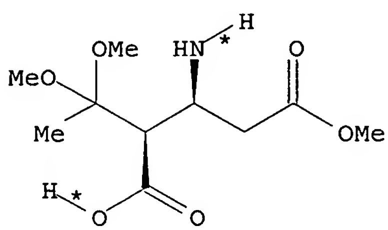


AB

(8) →



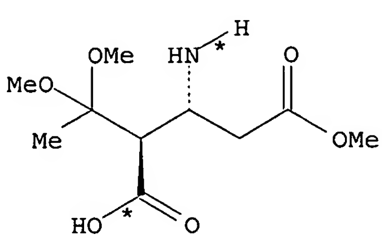
AC



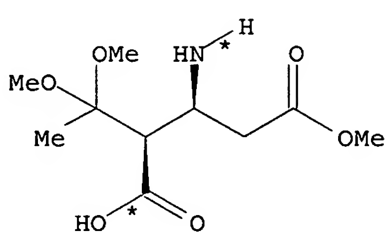
AD

RX(8)	RCT	AA 122313-70-6, AB 122313-71-7
	RGT	J 1333-74-0 H2
	PRO	AC 122313-59-1, AD 122313-60-4
	CAT	7440-05-3 Pd
	SOL	67-56-1 MeOH
	NTE	94% overall

RX(9) OF 100 ...AC + AD ===> AE + AF...

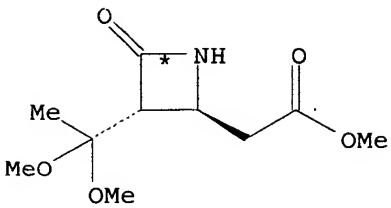


AC

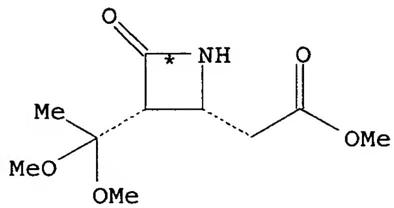


AD

(9) →



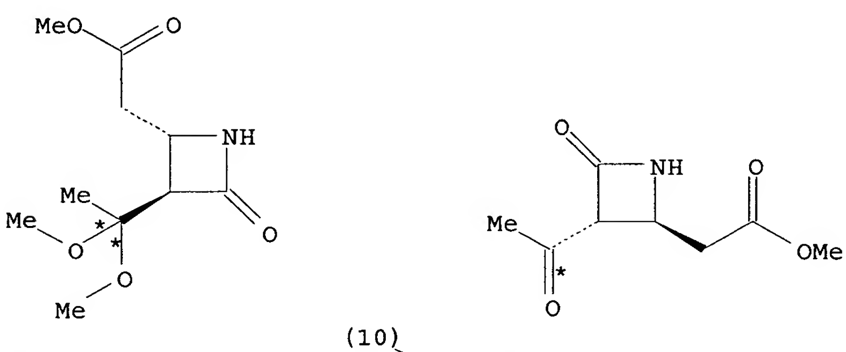
AE
YIELD 82%



AF
YIELD 15%

RX(9) RCT AC 122313-59-1, AD 122313-60-4
RGT Z 538-75-0 DCC
PRO AE 122313-61-5, AF 122313-62-6
SOL 109-99-9 THF

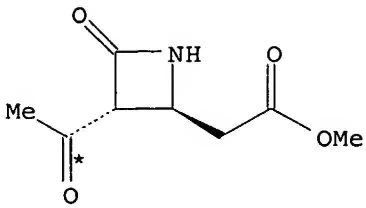
RX(10) OF 100 ...AE ===> AG...



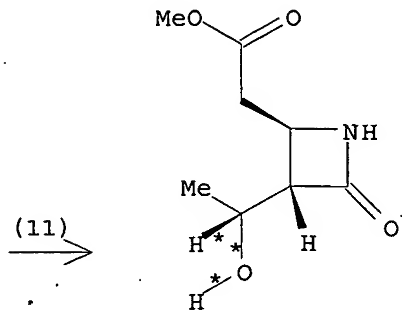
AE (10) AG

RX(10) RCT AE 122313-61-5
RGT AH 24057-28-1 Pyridinium tosylate
PRO AG 122313-63-7
SOL 67-64-1 Me2CO

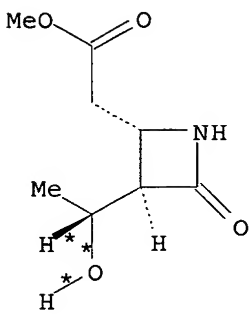
RX(11) OF 100 ...2 AG ===> AJ + AK...



2 AG



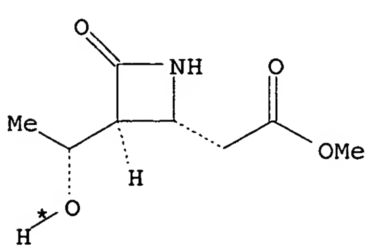
AJ
YIELD 95%(61)



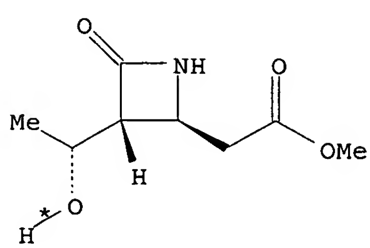
AK
YIELD 95%(39)

RX(11) RCT AG 122313-63-7
RGT AL 54575-49-4 K Selectride
PRO AJ 106248-39-9, AK 86421-11-6
SOL 109-99-9 THF

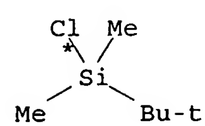
RX(12) OF 100 ...AJ + AK + 2 AM ===> AN + Y



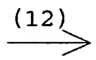
AJ

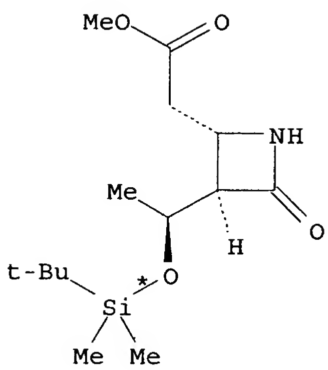


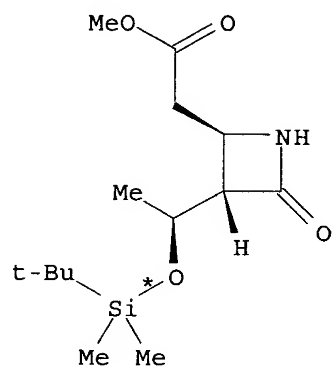
AK



2 AM





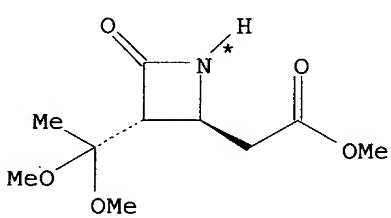


AN
YIELD 70%(61)

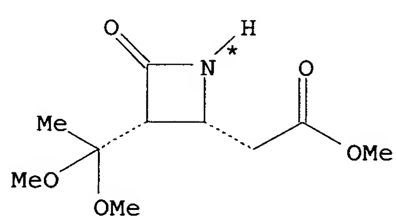
Y
YIELD 70%(39)

RX(12) RCT AJ 106248-39-9, AK 86421-11-6, AM 18162-48-6
RGT AO 288-32-4 1H-Imidazole
PRO AN 93711-82-1, Y 86421-12-7
SOL 68-12-2 DMF

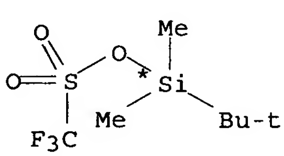
RX(13) OF 100 ...AE + AF + 2 AQ ===> AR + AS...



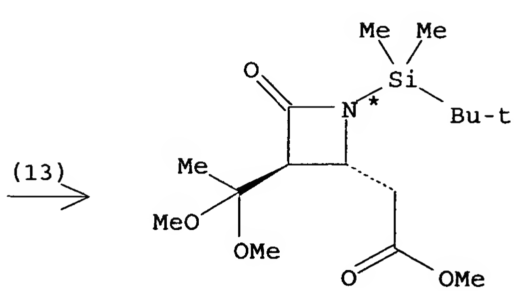
AE



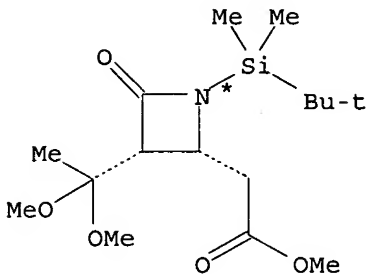
AF



2 AQ



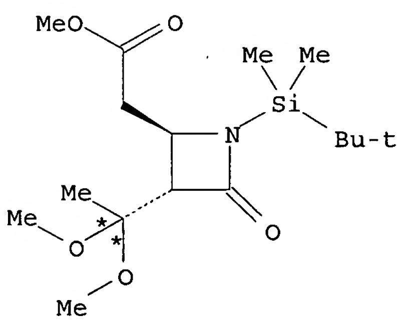
AR



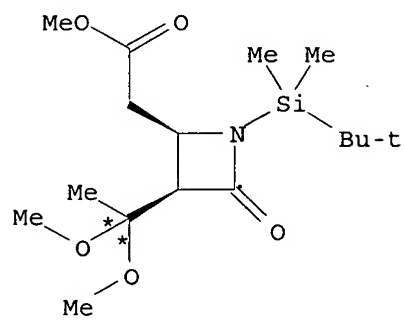
AS

RX(13)   RCT AE 122313-61-5, AF 122313-62-6, AQ 69739-34-0
           RGT AT 108-48-5 2,6-Lutidine
           PRO AR 122313-64-8, AS 122313-65-9
           SOL 75-09-2 CH2Cl2

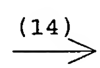
RX(14) OF 100   ...AR + AS ===> 2 AV...

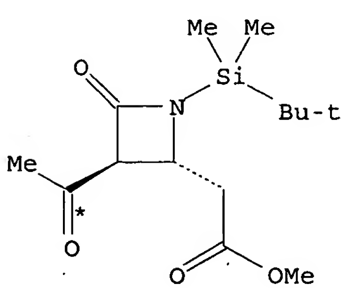


AR

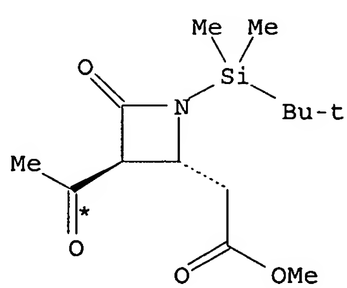


AS





AV
YIELD 100%

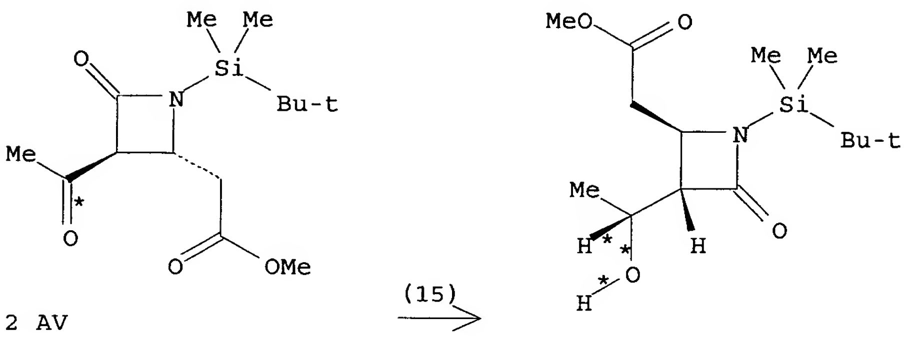


AV
YIELD 100%

RX(14)   RCT AR 122313-64-8, AS 122313-65-9

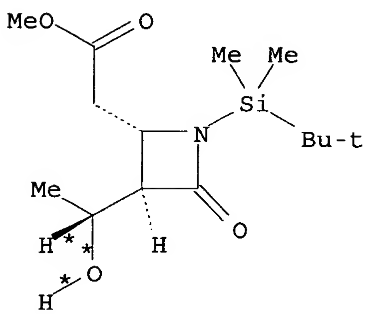
RGT AH 24057-28-1 Pyridinium tosylate
PRO AV 122332-75-6
SOL 67-64-1 Me2CO

RX(15) OF 100 ...2 AV ===> AW + AX



2 AV

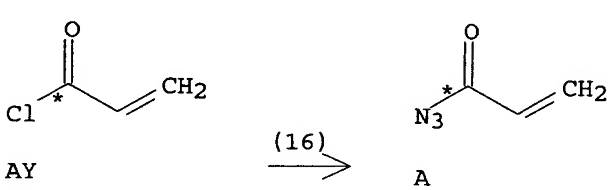
AW
YIELD 86%(50)



AX
YIELD 86%(50)

RX(15) RCT AV 122332-75-6
RGT AL 54575-49-4 K Selectride
PRO AW 122313-66-0, AX 122405-37-2
SOL 109-99-9 THF

RX(16) OF 100 AY ===> A...

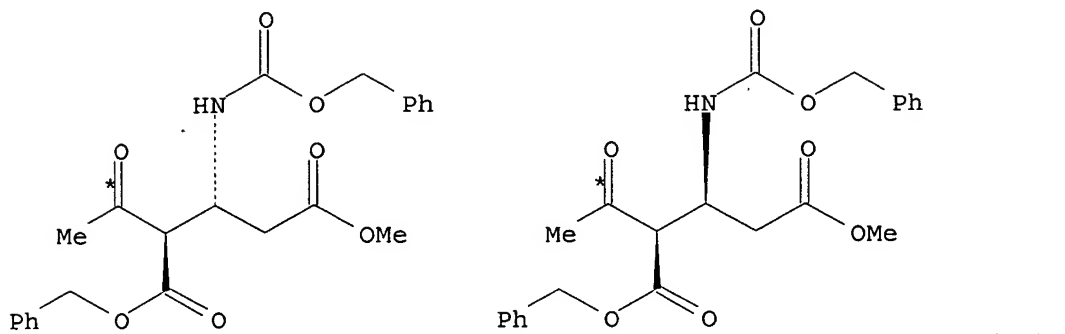


AY

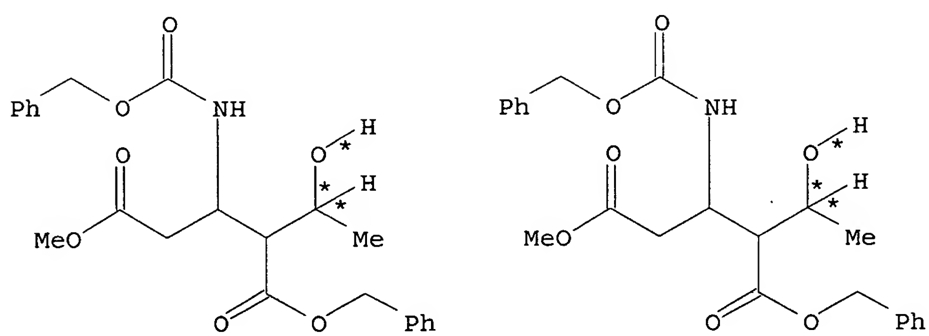
A

RX(16) RCT AY 814-68-6
RGT AZ 26628-22-8 NaN3
PRO A 50830-56-3
SOL 108-88-3 PhMe, 7732-18-5 Water

RX(17) OF 100 ...S + T ===> 2 BB...



S T

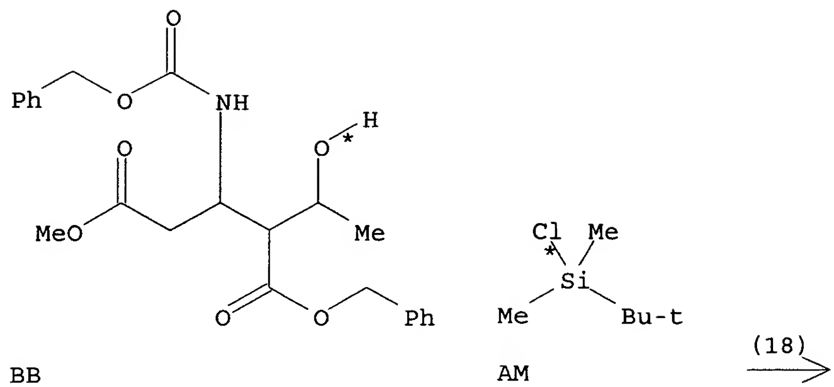


BB
YIELD 92%

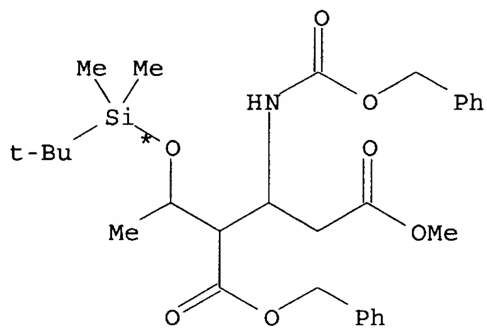
BB
YIELD 92%

RX(17) RCT S 122313-55-7, T 122313-56-8
RGT Q 16940-66-2 NaBH4
PRO BB 122313-68-2
SOL 67-56-1 MeOH

RX(18) OF 100 ...BB + AM ===> V...



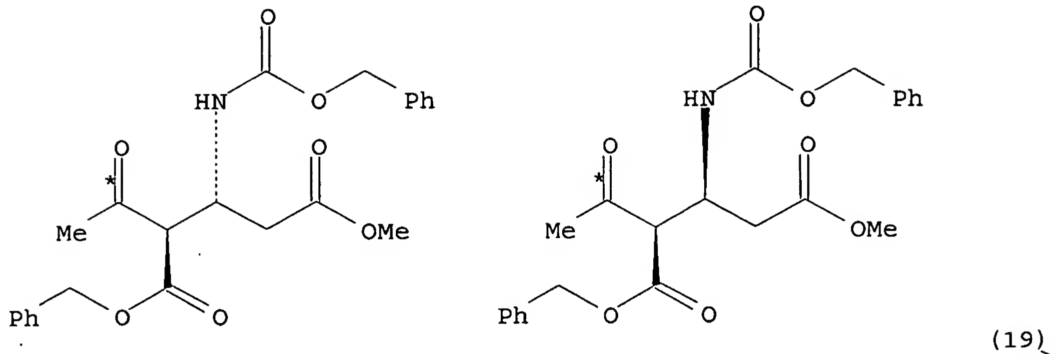
BB AM



V
YIELD 77%

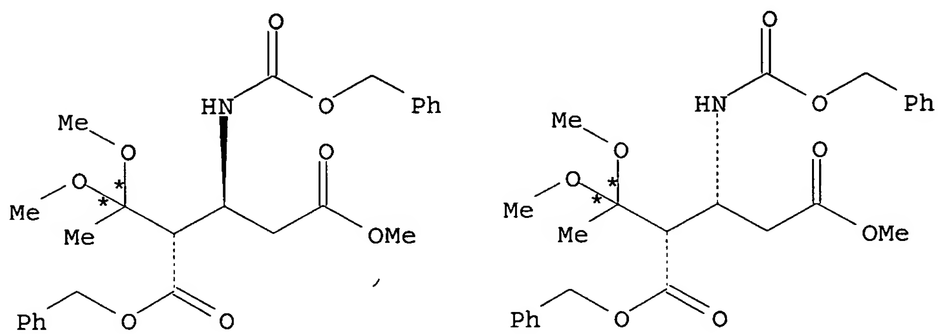
RX(18) RCT BB 122313-68-2, AM 18162-48-6
        RGT AO 288-32-4 1H-Imidazole
        PRO V 122313-69-3
        SOL 68-12-2 DMF

RX(19) OF 100 ...S + T ===> AA + AB...



S

T

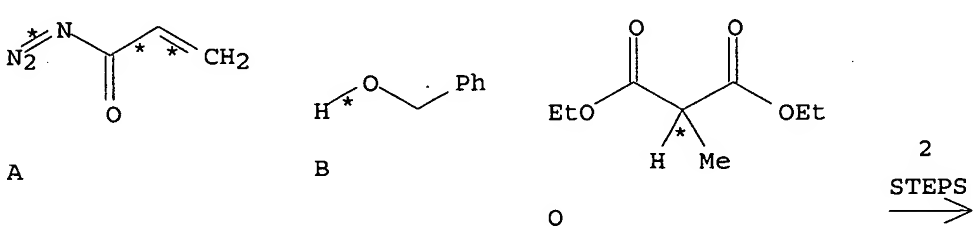


AA

AB

RX(19) RCT S 122313-55-7, T 122313-56-8
RGT BC 149-73-5 CH(OMe)3, BD 104-15-4 TsOH
PRO AA 122313-70-6, AB 122313-71-7
SOL 67-56-1 MeOH
NTE 90% overall

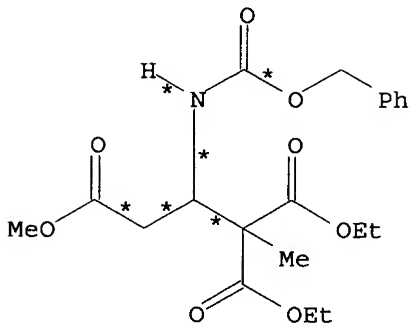
RX(22) OF 100 COMPOSED OF RX(1), RX(4)
RX(22) **A** + B + **O** ===> **P**



A

B

O



P
YIELD 63%

RX(1) RCT A **50830-56-3**, B 100-51-6
RGT D 123-31-9 Hydroquinone, E 110-86-1 Pyridine
PRO C 84713-20-2
SOL 108-88-3 PhMe

RX(4) RCT C 84713-20-2

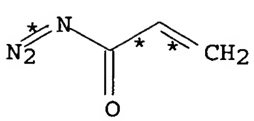
STAGE(1)
RGT H **14592-56-4** PdCl2(MeCN)2
SOL 109-99-9 THF

STAGE(2)
RCT O **609-08-5**
RGT Q 16940-66-2 NaBH4
SOL 109-99-9 THF

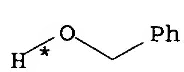
STAGE(3)
RGT I 121-44-8 Et3N
SOL 109-99-9 THF

PRO P **122313-54-6**

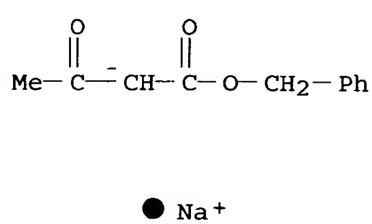
RX(23) OF 100 COMPOSED OF RX(1), RX(5)
RX(23) 2 **A** + 2 B + 2 **R** ===> **S** +
T



2 A

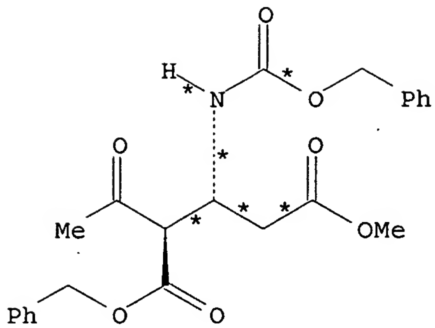


2 B

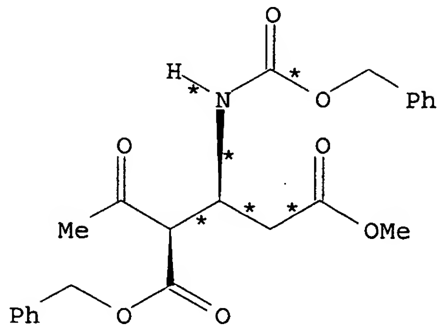


2 R

2 STEPS →



S
YIELD 92%(50)



T
YIELD 92%(50)

RX(1) RCT A **50830-56-3**, B 100-51-6
RGT D 123-31-9 Hydroquinone, E 110-86-1 Pyridine
PRO C 84713-20-2
SOL 108-88-3 PhMe

RX(5) RCT C 84713-20-2

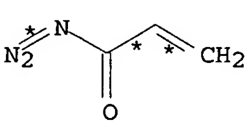
STAGE(1)
RGT H **14592-56-4** PdCl2(MeCN)2, I 121-44-8 Et3N
SOL 109-99-9 THF

STAGE(2)
RCT R **122313-67-1**
SOL 109-99-9 THF

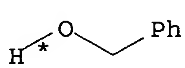
STAGE(3)
RGT K 67-56-1 MeOH, U 630-08-0 CO
SOL 109-99-9 THF, 67-56-1 MeOH

PRO S **122313-55-7**, T 122313-56-8

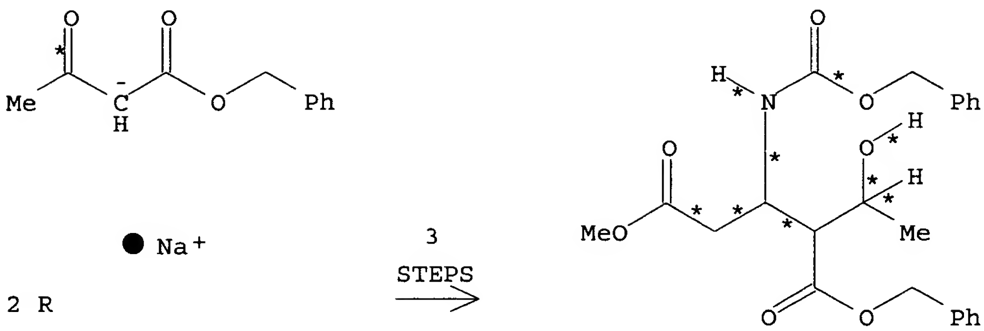
RX(38) OF 100 COMPOSED OF RX(1), RX(5), RX(17)
RX(38) 2 **A** + 2 B + 2 **R** ===> 2 **BB**



2 A

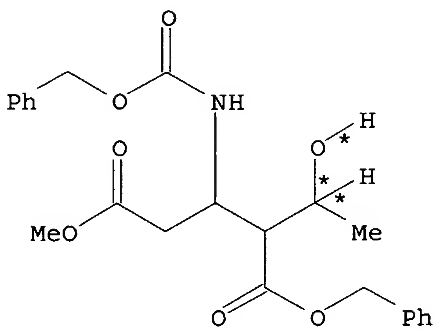


2 B



2 R

BB
YIELD 92%



BB
YIELD 92%

RX(1) RCT A **50830-56-3**, B 100-51-6
RGT D 123-31-9 Hydroquinone, E 110-86-1 Pyridine
PRO C 84713-20-2
SOL 108-88-3 PhMe

RX(5) RCT C 84713-20-2

STAGE(1)
RGT H **14592-56-4** PdCl2(MeCN)2, I 121-44-8 Et3N
SOL 109-99-9 THF

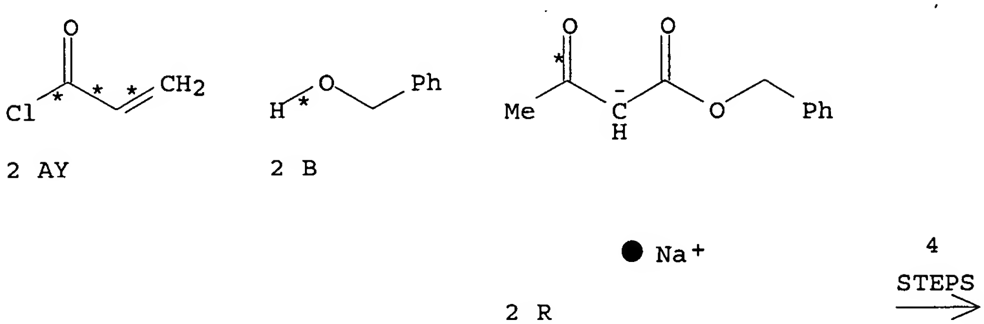
STAGE(2)
RCT R **122313-67-1**
SOL 109-99-9 THF

STAGE(3)
RGT K 67-56-1 MeOH, U 630-08-0 CO
SOL 109-99-9 THF, 67-56-1 MeOH

PRO S 122313-55-7, T 122313-56-8

RX(17) RCT S 122313-55-7, T 122313-56-8
RGT Q 16940-66-2 NaBH4
PRO BB **122313-68-2**
SOL 67-56-1 MeOH

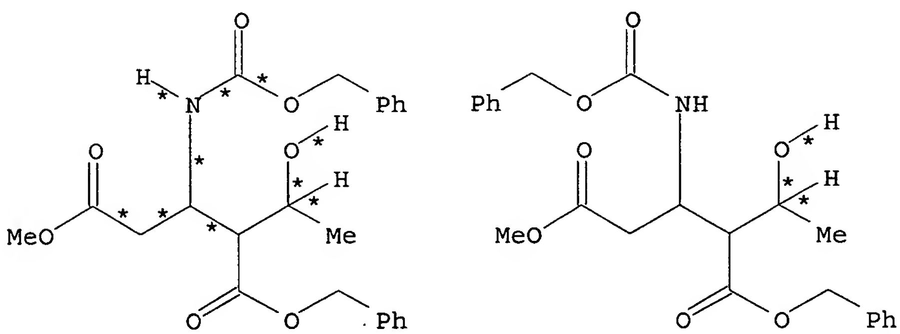
RX(40) OF 100 COMPOSED OF RX(16), RX(1), RX(5), RX(17)
RX(40) 2 **AY** + 2 B + 2 **R** ===> 2 **BB**



2 AY

2 B

2 R



BB
YIELD 92%

BB
YIELD 92%

RX(16) RCT AY **814-68-6**
RGT AZ 26628-22-8 NaN3
PRO A 50830-56-3
SOL 108-88-3 PhMe, 7732-18-5 Water

RX(1) RCT A 50830-56-3, B 100-51-6
RGT D 123-31-9 Hydroquinone, E 110-86-1 Pyridine
PRO C 84713-20-2
SOL 108-88-3 PhMe

RX(5) RCT C 84713-20-2

STAGE(1)
RGT H **14592-56-4** PdCl2(MeCN)2, I 121-44-8 Et3N
SOL 109-99-9 THF

STAGE(2)

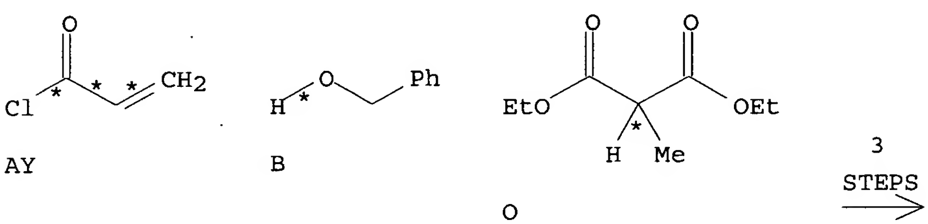
RCT R **122313-67-1**
SOL 109-99-9 THF

STAGE(3)
RGT K 67-56-1 MeOH, U 630-08-0 CO
SOL 109-99-9 THF, 67-56-1 MeOH

PRO S 122313-55-7, T 122313-56-8

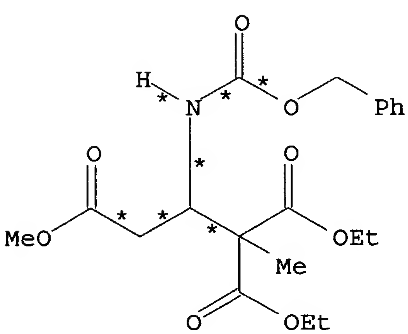
RX(17) RCT S 122313-55-7, T 122313-56-8
RGT Q 16940-66-2 NaBH4
PRO BB **122313-68-2**
SOL 67-56-1 MeOH

RX(60) OF 100 COMPOSED OF RX(16), RX(1), RX(4)
RX(60) **AY** + B + **O** ===> **P**



AY B O

3 STEPS



P
YIELD 63%

RX(16) RCT AY **814-68-6**
RGT AZ 26628-22-8 NaN3
PRO A 50830-56-3
SOL 108-88-3 PhMe, 7732-18-5 Water

RX(1) RCT A 50830-56-3, B 100-51-6
RGT D 123-31-9 Hydroquinone, E 110-86-1 Pyridine
PRO C 84713-20-2
SOL 108-88-3 PhMe

RX(4) RCT C 84713-20-2

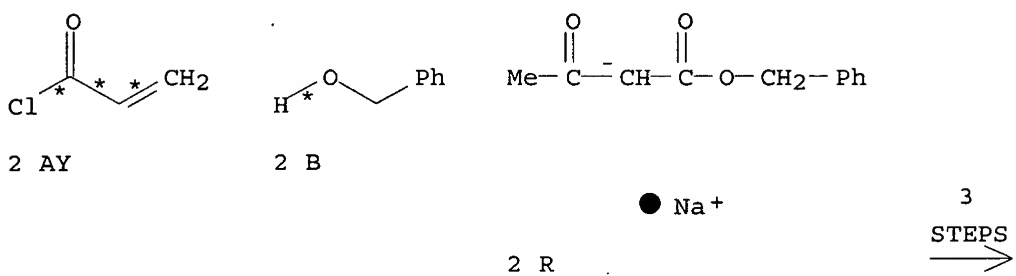
STAGE(1)
RGT H **14592-56-4** PdCl2(MeCN)2
SOL 109-99-9 THF

STAGE(2)
RCT O **609-08-5**
RGT Q 16940-66-2 NaBH4
SOL 109-99-9 THF

STAGE(3)
RGT I 121-44-8 Et3N
SOL 109-99-9 THF

PRO P **122313-54-6**

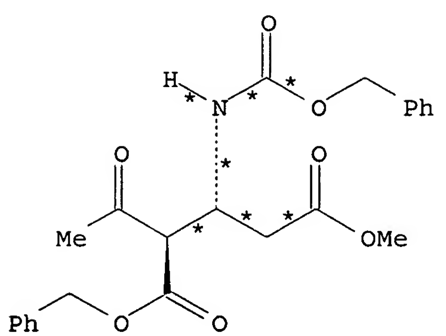
RX(61) OF 100 COMPOSED OF RX(16), RX(1), RX(5)
RX(61) 2 **AY** + 2 B + 2 **R** ===> **S** + T



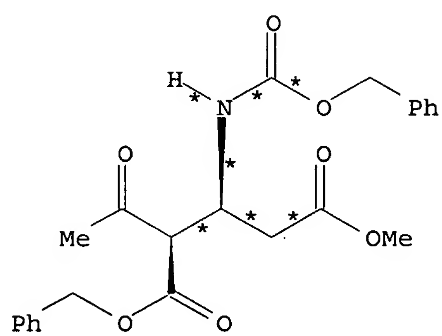
2 AY

2 B

2 R



S
YIELD 92%(50)

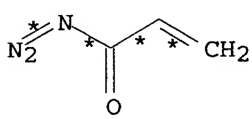


T
YIELD 92%(50)

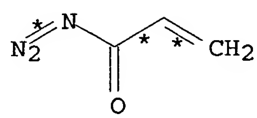
RX(16) RCT AY **814-68-6**
RGT AZ 26628-22-8 NaN3
PRO A 50830-56-3
SOL 108-88-3 PhMe, 7732-18-5 Water

RX(1) RCT A 50830-56-3, B 100-51-6
RGT D 123-31-9 Hydroquinone, E 110-86-1 Pyridine

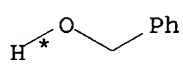
```
          PRO   C 84713-20-2
          SOL   108-88-3 PhMe

RX(5)     RCT   C 84713-20-2

            STAGE(1)
               RGT   H 14592-56-4 PdCl2(MeCN)2, I 121-44-8
                     Et3N
               SOL   109-99-9 THF

            STAGE(2)
               RCT   R 122313-67-1
               SOL   109-99-9 THF

            STAGE(3)
               RGT   K 67-56-1 MeOH, U 630-08-0 CO
               SOL   109-99-9 THF, 67-56-1 MeOH

          PRO   S 122313-55-7, T 122313-56-8


RX(77) OF 100 COMPOSED OF RX(1), RX(5), RX(19), RX(8), RX(9), RX(10)
RX(77)    2 A  +  2 B  +  2 R  ===>  AG
```



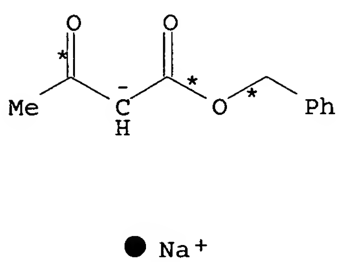
A



A



2 B



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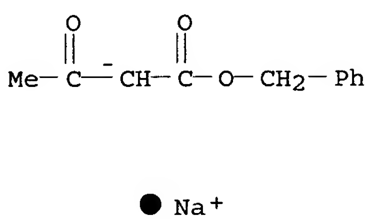
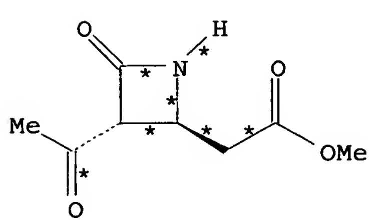


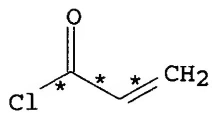
R

6 STEPS →

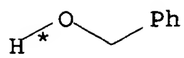


AG

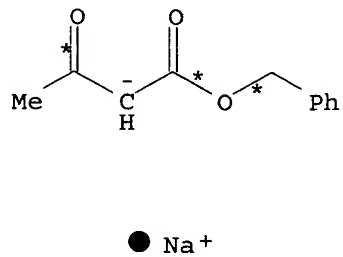
```
RX(1)       RCT  A 50830-56-3, B 100-51-6
            RGT  D 123-31-9 Hydroquinone, E 110-86-1 Pyridine
            PRO  C 84713-20-2
            SOL  108-88-3 PhMe

RX(5)       RCT  C 84713-20-2

              STAGE(1)
                 RGT  H 14592-56-4 PdCl2(MeCN)2, I 121-44-8
                      Et3N
                 SOL  109-99-9 THF

              STAGE(2)
                 RCT  R 122313-67-1
                 SOL  109-99-9 THF

              STAGE(3)
                 RGT  K 67-56-1 MeOH, U 630-08-0 CO
                 SOL  109-99-9 THF, 67-56-1 MeOH

            PRO  S 122313-55-7, T 122313-56-8

RX(19)      RCT  S 122313-55-7, T 122313-56-8
            RGT  BC 149-73-5 CH(OMe)3, BD 104-15-4 TsOH
            PRO  AA 122313-70-6, AB 122313-71-7
            SOL  67-56-1 MeOH
            NTE  90% overall

RX(8)       RCT  AA 122313-70-6, AB 122313-71-7
            RGT  J 1333-74-0 H2
            PRO  AC 122313-59-1, AD 122313-60-4
            CAT  7440-05-3 Pd
            SOL  67-56-1 MeOH
            NTE  94% overall

RX(9)       RCT  AC 122313-59-1, AD 122313-60-4
            RGT  Z 538-75-0 DCC
            PRO  AE 122313-61-5, AF 122313-62-6
            SOL  109-99-9 THF

RX(10)      RCT  AE 122313-61-5
            RGT  AH 24057-28-1 Pyridinium tosylate
            PRO  AG 122313-63-7
            SOL  67-64-1 Me2CO


RX(80) OF 100 COMPOSED OF RX(16), RX(1), RX(5), RX(19), RX(8), RX(9),
            RX(10)
RX(80)      2 AY  +  2 B  +  2 R  ===>  AG
```



2 AY



2 B



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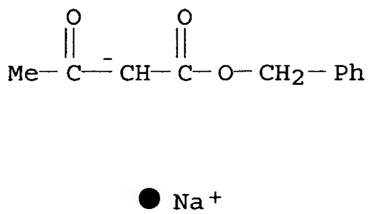
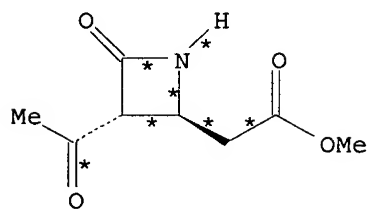


R

7

STEPS

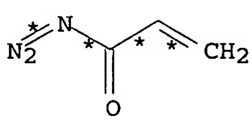
⟹



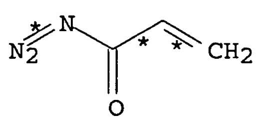
AG

```
RX(16)     RCT   AY 814-68-6
           RGT   AZ 26628-22-8 NaN3
           PRO   A 50830-56-3
           SOL   108-88-3 PhMe, 7732-18-5 Water

RX(1)      RCT   A 50830-56-3, B 100-51-6
           RGT   D 123-31-9 Hydroquinone, E 110-86-1 Pyridine
           PRO   C 84713-20-2
           SOL   108-88-3 PhMe

RX(5)      RCT   C 84713-20-2

             STAGE(1)
                RGT   H 14592-56-4 PdCl2(MeCN)2, I 121-44-8
                      Et3N
                SOL   109-99-9 THF

             STAGE(2)
                RCT   R 122313-67-1
                SOL   109-99-9 THF

             STAGE(3)
                RGT   K 67-56-1 MeOH, U 630-08-0 CO
                SOL   109-99-9 THF, 67-56-1 MeOH

           PRO   S 122313-55-7, T 122313-56-8

RX(19)     RCT   S 122313-55-7, T 122313-56-8
           RGT   BC 149-73-5 CH(OMe)3, BD 104-15-4 TsOH
           PRO   AA 122313-70-6, AB 122313-71-7
           SOL   67-56-1 MeOH
           NTE   90% overall
```

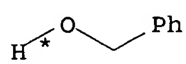
```
RX(8)       RCT  AA 122313-70-6, AB 122313-71-7
            RGT  J 1333-74-0 H2
            PRO  AC 122313-59-1, AD 122313-60-4
            CAT  7440-05-3 Pd
            SOL  67-56-1 MeOH
            NTE  94% overall

RX(9)       RCT  AC 122313-59-1, AD 122313-60-4
            RGT  Z 538-75-0 DCC
            PRO  AE 122313-61-5, AF 122313-62-6
            SOL  109-99-9 THF

RX(10)      RCT  AE 122313-61-5
            RGT  AH 24057-28-1 Pyridinium tosylate
            PRO  AG 122313-63-7
            SOL  67-64-1 Me2CO


RX(93) OF 100 COMPOSED OF RX(1), RX(5), RX(19), RX(8), RX(9), RX(10),
            RX(11)
RX(93)      3 A  +  B  +  3 R  ===>  AJ  +
            AK
```



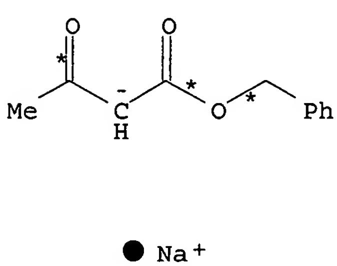
2 A



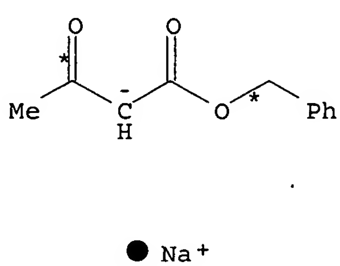
A



B



R



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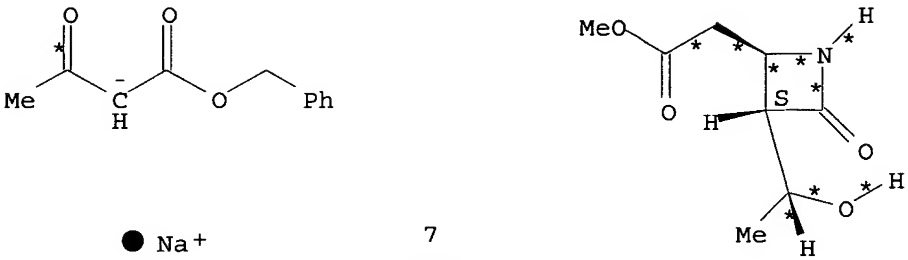
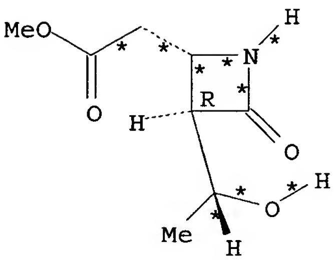


R

7
STEPS
⟶

AJ
YIELD 95%(61)



AK
YIELD 95%(39)

RX(1) RCT A **50830-56-3**, B 100-51-6
RGT D 123-31-9 Hydroquinone, E 110-86-1 Pyridine
PRO C 84713-20-2
SOL 108-88-3 PhMe

RX(5) RCT C 84713-20-2

STAGE(1)
RGT H **14592-56-4** PdCl2(MeCN)2, I 121-44-8 Et3N
SOL 109-99-9 THF

STAGE(2)
RCT R **122313-67-1**
SOL 109-99-9 THF

STAGE(3)
RGT K 67-56-1 MeOH, U 630-08-0 CO
SOL 109-99-9 THF, 67-56-1 MeOH

PRO S 122313-55-7, T 122313-56-8

RX(19) RCT S 122313-55-7, T 122313-56-8
RGT BC 149-73-5 CH(OMe)3, BD 104-15-4 TsOH
PRO AA 122313-70-6, AB 122313-71-7
SOL 67-56-1 MeOH
NTE 90% overall

RX(8) RCT AA 122313-70-6, AB 122313-71-7
RGT J 1333-74-0 H2
PRO AC 122313-59-1, AD 122313-60-4
CAT 7440-05-3 Pd
SOL 67-56-1 MeOH
NTE 94% overall

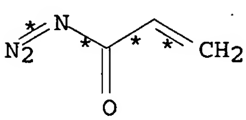
RX(9) RCT AC 122313-59-1, AD 122313-60-4
RGT Z 538-75-0 DCC
PRO AE 122313-61-5, AF 122313-62-6
SOL 109-99-9 THF

RX(10) RCT AE 122313-61-5
RGT AH 24057-28-1 Pyridinium tosylate
PRO AG 122313-63-7
SOL 67-64-1 Me2CO

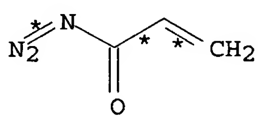
RX(11) RCT AG 122313-63-7
RGT AL 54575-49-4 K Selectride
PRO AJ **106248-39-9**, AK 86421-11-6
SOL 109-99-9 THF

RX(94) OF 100 COMPOSED OF RX(1), RX(5), RX(19), RX(8), RX(9), RX(13), RX(14)

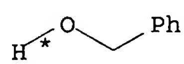
RX(94) 2 **A** + B + 2 **R** + 2 AQ ===> 2 **AV**



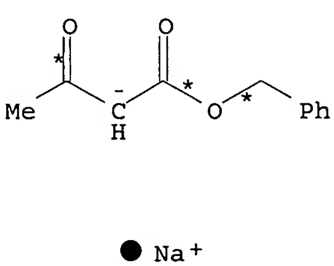
A



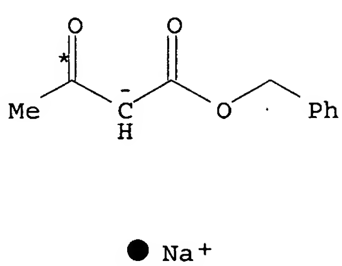
A



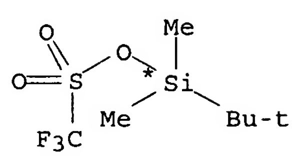
B



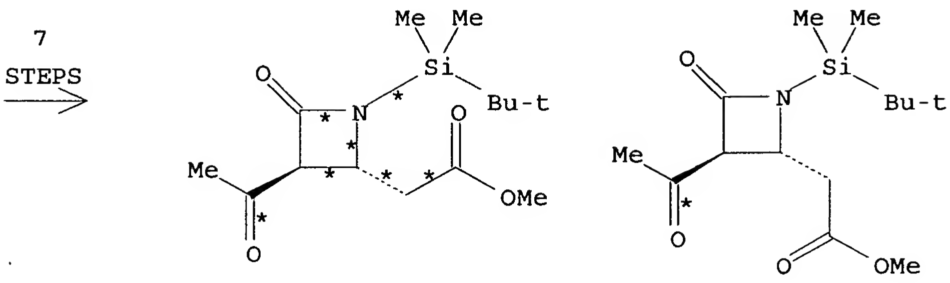
R



R



2 AQ



AV
YIELD 100%

AV
YIELD 100%

RX(1) RCT A **50830-56-3**, B 100-51-6
RGT D 123-31-9 Hydroquinone, E 110-86-1 Pyridine
PRO C 84713-20-2
SOL 108-88-3 PhMe

RX(5) RCT C 84713-20-2

STAGE(1)
RGT H **14592-56-4** PdCl2(MeCN)2, I 121-44-8 Et3N
SOL 109-99-9 THF

STAGE(2)
RCT R **122313-67-1**
SOL 109-99-9 THF

STAGE(3)
RGT K 67-56-1 MeOH, U 630-08-0 CO
SOL 109-99-9 THF, 67-56-1 MeOH

PRO S 122313-55-7, T 122313-56-8

RX(19) RCT S 122313-55-7, T 122313-56-8
RGT BC 149-73-5 CH(OMe)3, BD 104-15-4 TsOH
PRO AA 122313-70-6, AB 122313-71-7
SOL 67-56-1 MeOH
NTE 90% overall

RX(8) RCT AA 122313-70-6, AB 122313-71-7
RGT J 1333-74-0 H2
PRO AC 122313-59-1, AD 122313-60-4
CAT 7440-05-3 Pd
SOL 67-56-1 MeOH
NTE 94% overall

RX(9) RCT AC 122313-59-1, AD 122313-60-4
RGT Z 538-75-0 DCC
PRO AE 122313-61-5, AF 122313-62-6
SOL 109-99-9 THF

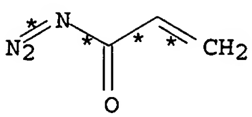
RX(13) RCT AE 122313-61-5, AF 122313-62-6, AQ 69739-34-0
RGT AT 108-48-5 2,6-Lutidine
PRO AR 122313-64-8, AS 122313-65-9

SOL 75-09-2 CH2Cl2

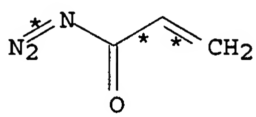
RX(14) RCT AR 122313-64-8, AS 122313-65-9
RGT AH 24057-28-1 Pyridinium tosylate
PRO AV **122332-75-6**
SOL 67-64-1 Me2CO

RX(96) OF 100 COMPOSED OF RX(1), RX(5), RX(19), RX(8), RX(9), RX(13), RX(14), RX(15)

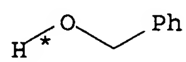
RX(96) 3 **A** + B + 3 **R** + 3 AQ ===>
AW + AX



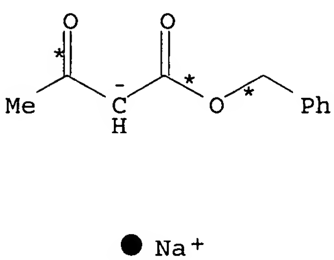
2 A



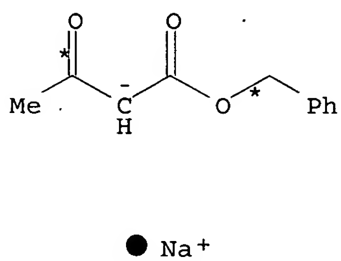
A



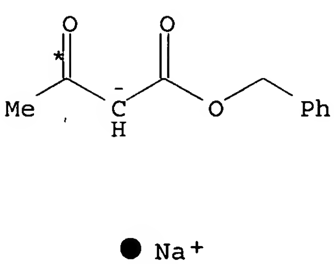
B



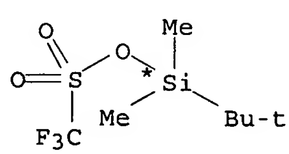
R



R

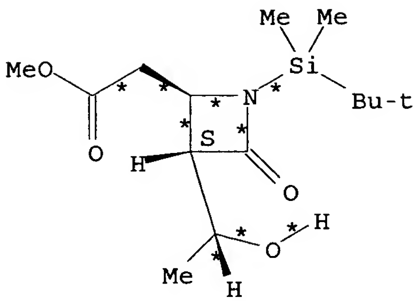


R

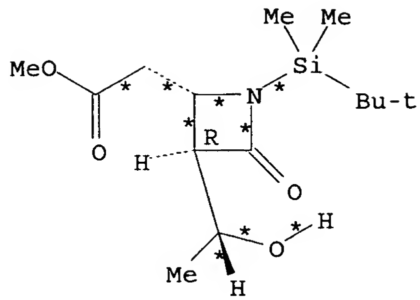


3 AQ

8 STEPS →



AW
YIELD 86%(50)



AX
YIELD 86%(50)

RX(1) RCT A **50830-56-3**, B 100-51-6
RGT D 123-31-9 Hydroquinone, E 110-86-1 Pyridine
PRO C 84713-20-2
SOL 108-88-3 PhMe

RX(5) RCT C 84713-20-2

STAGE(1)
RGT H **14592-56-4** PdCl2(MeCN)2, I 121-44-8 Et3N
SOL 109-99-9 THF

STAGE(2)
RCT R **122313-67-1**
SOL 109-99-9 THF

STAGE(3)
RGT K 67-56-1 MeOH, U 630-08-0 CO
SOL 109-99-9 THF, 67-56-1 MeOH

PRO S 122313-55-7, T 122313-56-8

RX(19) RCT S 122313-55-7, T 122313-56-8
RGT BC 149-73-5 CH(OMe)3, BD 104-15-4 TsOH
PRO AA 122313-70-6, AB 122313-71-7
SOL 67-56-1 MeOH
NTE 90% overall

RX(8) RCT AA 122313-70-6, AB 122313-71-7
RGT J 1333-74-0 H2
PRO AC 122313-59-1, AD 122313-60-4
CAT 7440-05-3 Pd
SOL 67-56-1 MeOH
NTE 94% overall

RX(9) RCT AC 122313-59-1, AD 122313-60-4
RGT Z 538-75-0 DCC
PRO AE 122313-61-5, AF 122313-62-6
SOL 109-99-9 THF

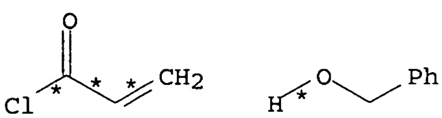
RX(13) RCT AE 122313-61-5, AF 122313-62-6, AQ 69739-34-0
RGT AT 108-48-5 2,6-Lutidine

PRO AR 122313-64-8, AS 122313-65-9
SOL 75-09-2 CH2Cl2

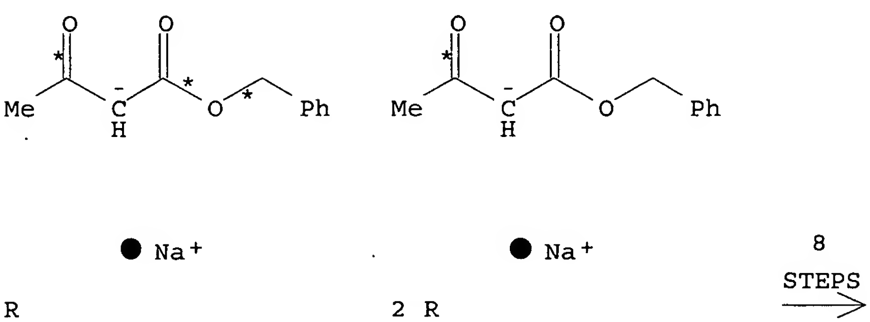
RX(14) RCT AR 122313-64-8, AS 122313-65-9
RGT AH 24057-28-1 Pyridinium tosylate
PRO AV 122332-75-6
SOL 67-64-1 Me2CO

RX(15) RCT AV 122332-75-6
RGT AL 54575-49-4 K Selectride
PRO AW **122313-66-0**, AX 122405-37-2
SOL 109-99-9 THF

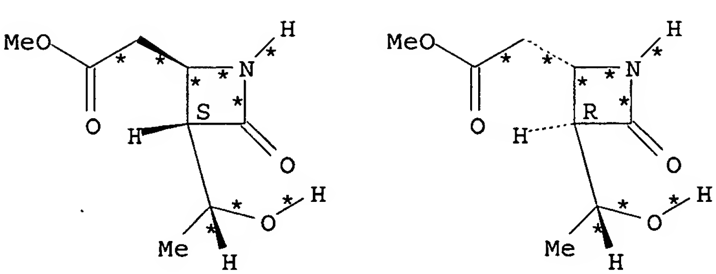
RX(97) OF 100 COMPOSED OF RX(16), RX(1), RX(5), RX(19), RX(8), RX(9), RX(10), RX(11)
RX(97) 3 **AY** + 3 B + 3 **R** ===> **AJ** + AK



3 AY 3 B



R 2 R

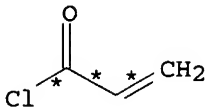


AJ
YIELD 95%(61)

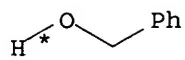
AK
YIELD 95%(39)

RX(16) RCT AY **814-68-6**
RGT AZ 26628-22-8 NaN3

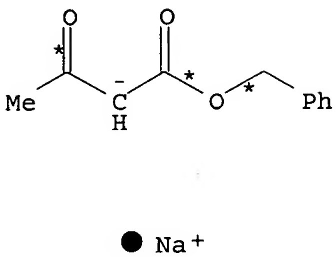
```
          PRO  A 50830-56-3
          SOL  108-88-3 PhMe, 7732-18-5 Water

RX(1)     RCT  A 50830-56-3, B 100-51-6
          RGT  D 123-31-9 Hydroquinone, E 110-86-1 Pyridine
          PRO  C 84713-20-2
          SOL  108-88-3 PhMe

RX(5)     RCT  C 84713-20-2

            STAGE(1)
               RGT  H 14592-56-4 PdCl2(MeCN)2, I 121-44-8
                    Et3N
               SOL  109-99-9 THF

            STAGE(2)
               RCT  R 122313-67-1
               SOL  109-99-9 THF

            STAGE(3)
               RGT  K 67-56-1 MeOH, U 630-08-0 CO
               SOL  109-99-9 THF, 67-56-1 MeOH

          PRO  S 122313-55-7, T 122313-56-8

RX(19)    RCT  S 122313-55-7, T 122313-56-8
          RGT  BC 149-73-5 CH(OMe)3, BD 104-15-4 TsOH
          PRO  AA 122313-70-6, AB 122313-71-7
          SOL  67-56-1 MeOH
          NTE  90% overall

RX(8)     RCT  AA 122313-70-6, AB 122313-71-7
          RGT  J 1333-74-0 H2
          PRO  AC 122313-59-1, AD 122313-60-4
          CAT  7440-05-3 Pd
          SOL  67-56-1 MeOH
          NTE  94% overall

RX(9)     RCT  AC 122313-59-1, AD 122313-60-4
          RGT  Z 538-75-0 DCC
          PRO  AE 122313-61-5, AF 122313-62-6
          SOL  109-99-9 THF

RX(10)    RCT  AE 122313-61-5
          RGT  AH 24057-28-1 Pyridinium tosylate
          PRO  AG 122313-63-7
          SOL  67-64-1 Me2CO

RX(11)    RCT  AG 122313-63-7
          RGT  AL 54575-49-4 K Selectride
          PRO  AJ 106248-39-9, AK 86421-11-6
          SOL  109-99-9 THF


RX(98) OF 100 COMPOSED OF RX(16), RX(1), RX(5), RX(19), RX(8), RX(9),
          RX(13), RX(14)
RX(98)    2 AY  +  2 B  +  2 R  +  2 AQ  ===>  2
          AV
```



2 AY



2 B



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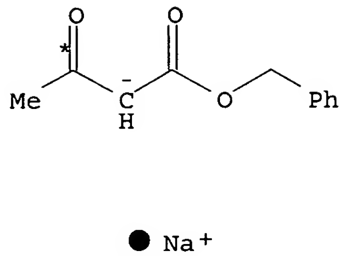

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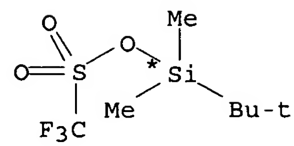
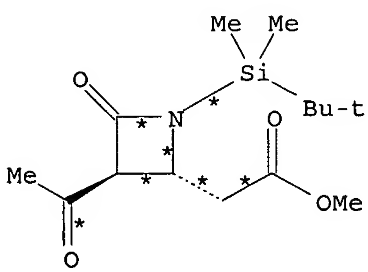
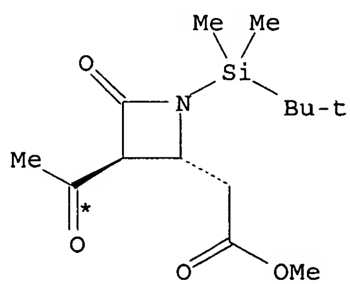


2 AQ

8
STEPS



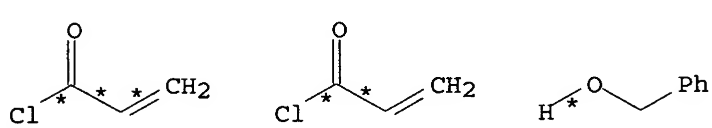
AV
YIELD 100%



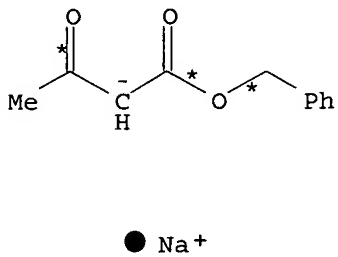
AV
YIELD 100%

```
RX(16)     RCT  AY 814-68-6
           RGT  AZ 26628-22-8 NaN3
           PRO  A 50830-56-3
           SOL  108-88-3 PhMe, 7732-18-5 Water

RX(1)      RCT  A 50830-56-3, B 100-51-6
           RGT  D 123-31-9 Hydroquinone, E 110-86-1 Pyridine
           PRO  C 84713-20-2
           SOL  108-88-3 PhMe

RX(5)      RCT  C 84713-20-2

             STAGE(1)
                RGT  H 14592-56-4 PdCl2(MeCN)2, I 121-44-8
```

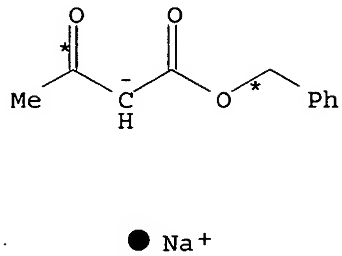
```
            Et3N
        SOL  109-99-9 THF

     STAGE(2)
        RCT  R 122313-67-1
        SOL  109-99-9 THF

     STAGE(3)
        RGT  K 67-56-1 MeOH, U 630-08-0 CO
        SOL  109-99-9 THF, 67-56-1 MeOH

      PRO  S 122313-55-7, T 122313-56-8

RX(19)  RCT  S 122313-55-7, T 122313-56-8
        RGT  BC 149-73-5 CH(OMe)3, BD 104-15-4 TsOH
        PRO  AA 122313-70-6, AB 122313-71-7
        SOL  67-56-1 MeOH
        NTE  90% overall

RX(8)   RCT  AA 122313-70-6, AB 122313-71-7
        RGT  J 1333-74-0 H2
        PRO  AC 122313-59-1, AD 122313-60-4
        CAT  7440-05-3 Pd
        SOL  67-56-1 MeOH
        NTE  94% overall

RX(9)   RCT  AC 122313-59-1, AD 122313-60-4
        RGT  Z 538-75-0 DCC
        PRO  AE 122313-61-5, AF 122313-62-6
        SOL  109-99-9 THF

RX(13)  RCT  AE 122313-61-5, AF 122313-62-6, AQ 69739-34-0
        RGT  AT 108-48-5 2,6-Lutidine
        PRO  AR 122313-64-8, AS 122313-65-9
        SOL  75-09-2 CH2Cl2

RX(14)  RCT  AR 122313-64-8, AS 122313-65-9
        RGT  AH 24057-28-1 Pyridinium tosylate
        PRO  AV 122332-75-6
        SOL  67-64-1 Me2CO


RX(100) OF 100 COMPOSED OF RX(16), RX(1), RX(5), RX(19), RX(8), RX(9),
        RX(13), RX(14), RX(15)
RX(100)   3 AY  +  3 B  +  3 R  +  3 AQ  ===>
          AW  +  AX
```



2 AY   AY   3 B



R



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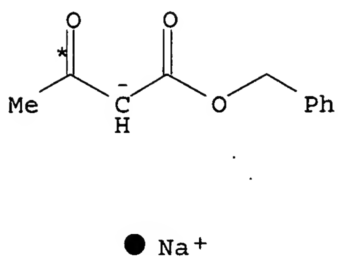

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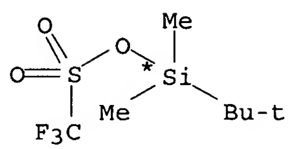
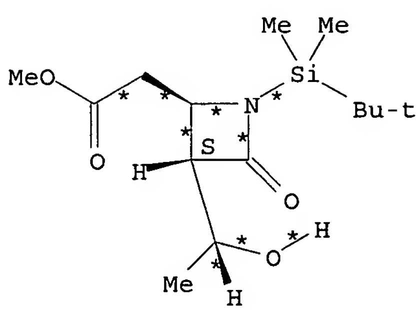
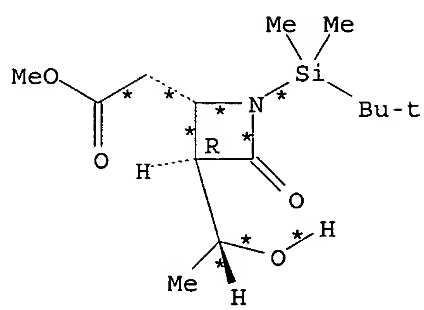


3 AQ

9 STEPS



AW
YIELD 86%(50)



AX
YIELD 86%(50)

RX(16) RCT AY **814-68-6**
RGT AZ 26628-22-8 NaN3
PRO A 50830-56-3
SOL 108-88-3 PhMe, 7732-18-5 Water

RX(1) RCT A 50830-56-3, B 100-51-6
RGT D 123-31-9 Hydroquinone, E 110-86-1 Pyridine
PRO C 84713-20-2
SOL 108-88-3 PhMe

RX(5) RCT C 84713-20-2

```
   STAGE(1)
      RGT  H 14592-56-4 PdCl2(MeCN)2, I 121-44-8
           Et3N
      SOL  109-99-9 THF

   STAGE(2)
      RCT  R 122313-67-1
      SOL  109-99-9 THF

   STAGE(3)
      RGT  K 67-56-1 MeOH, U 630-08-0 CO
      SOL  109-99-9 THF, 67-56-1 MeOH

  PRO  S 122313-55-7, T 122313-56-8

RX(19)    RCT  S 122313-55-7, T 122313-56-8
          RGT  BC 149-73-5 CH(OMe)3, BD 104-15-4 TsOH
          PRO  AA 122313-70-6, AB 122313-71-7
          SOL  67-56-1 MeOH
          NTE  90% overall

RX(8)     RCT  AA 122313-70-6, AB 122313-71-7
          RGT  J 1333-74-0 H2
          PRO  AC 122313-59-1, AD 122313-60-4
          CAT  7440-05-3 Pd
          SOL  67-56-1 MeOH
          NTE  94% overall

RX(9)     RCT  AC 122313-59-1, AD 122313-60-4
          RGT  Z 538-75-0 DCC
          PRO  AE 122313-61-5, AF 122313-62-6
          SOL  109-99-9 THF

RX(13)    RCT  AE 122313-61-5, AF 122313-62-6, AQ 69739-34-0
          RGT  AT 108-48-5 2,6-Lutidine
          PRO  AR 122313-64-8, AS 122313-65-9
          SOL  75-09-2 CH2Cl2

RX(14)    RCT  AR 122313-64-8, AS 122313-65-9
          RGT  AH 24057-28-1 Pyridinium tosylate
          PRO  AV 122332-75-6
          SOL  67-64-1 Me2CO

RX(15)    RCT  AV 122332-75-6
          RGT  AL 54575-49-4 K Selectride
          PRO  AW 122313-66-0, AX 122405-37-2
          SOL  109-99-9 THF
```

L20 ANSWER 6 OF 7 CASREACT COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 109:170611 CASREACT

TITLE: Diversity in modes of reactions of [η3-1-(trimethylsiloxy)allyl]iron dicarbonyl nitronyl complexes. Nucleophilic addition and cyclization of the allylic ligands

AUTHOR(S): Ito, Keiji; Nakanishi, Saburo; Otsuji, Yoshio

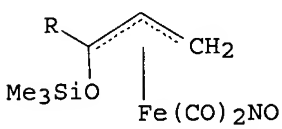
CORPORATE SOURCE: Dep. Ind. Chem., Osaka Prefect. Coll. Technol., Osaka, 572, Japan

SOURCE: Chemistry Letters (1988), (3), 473-6

CODEN: CMLTAG; ISSN: 0366-7022

DOCUMENT TYPE: Journal
LANGUAGE: English
CLASSIFICATION: 29-12 (Organometallic and Organometalloidal Compounds)
Section cross-reference(s): 23, 25, 27

GRAPHIC IMAGE:



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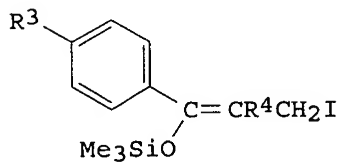

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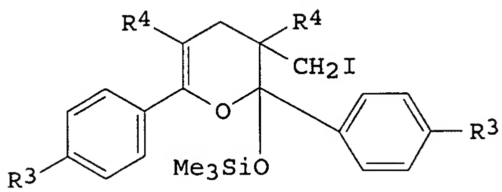


III

ABSTRACT:
The title iron complexes (I; R = Ph, Et, OMe) derived from Me3SiOCR:CHCH2I and [Bu4N][Fe(CO)3NO] reacted with carbon nucleophiles such as NaCH(CO2Et)2 to give RCOCH2CH2CHR1R2 (same R; R1 = R2 = CO2Et, cyano; R1 = Ac, R2 = CO2Et) in 42-95% yields. The addition occurred at the 3-position of the ligands with high regioselectivity. However, the iron complexes derived from 2-alkyl-3-iodo-1-trimethylsiloxypropenes II (R3 = H, Me, OMe, Cl; R4 = Me, Et) underwent cyclization reaction with the same siloxypropenes to give dihydropyran derivs. III.

SUPPL. TERM: methylsiloxyallyliron dicarbonyl nitrosyl complex addn; cyclization allylic ligand; pyran siloxyiodomethylphenyl; iron complex addn nucleophile regiochem

INDEX TERM: Regiochemistry
(of addition reaction of iodosiloxypropenes with carbonylnitrosoiron complex)

INDEX TERM: Addition reaction
(of iodosiloxypropenes with carbonylnitrosoiron complex)

INDEX TERM: 96206-23-4
ROLE: RCT (Reactant); RACT (Reactant or reagent)
(addition reaction of, with iodosilyloxypropenes)

INDEX TERM: 670-80-4 996-82-7 20334-42-3 34284-28-1
ROLE: RCT (Reactant); RACT (Reactant or reagent)
(addition reaction of, with iron complexes)

INDEX TERM: 116309-64-9
ROLE: RCT (Reactant); RACT (Reactant or reagent)
(addition reaction of, with nucleophiles)

INDEX TERM: 96-33-3, Methyl acrylate 768-03-6, Phenyl vinyl ketone 769-60-8 1629-58-9, Ethyl vinyl ketone 6230-72-4 6230-73-5 22731-65-3 62834-89-3
ROLE: RCT (Reactant); RACT (Reactant or reagent)
(iodosilylation of)

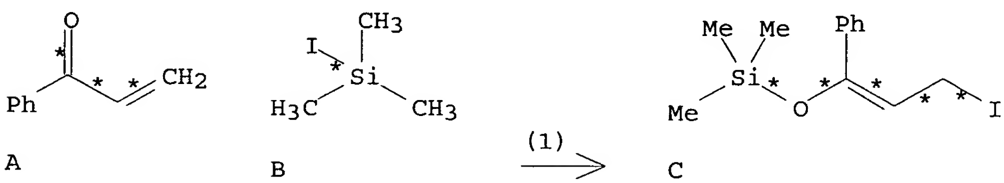
INDEX TERM: 116981-02-3P 116981-03-4P 116981-04-5P
116981-05-6P 116981-06-7P
ROLE: RCT (Reactant); SPN (Synthetic preparation);
PREP (Preparation); RACT (Reactant or reagent)
(preparation and addition reaction of, with iron
complexes)

INDEX TERM: 116309-63-8P 116309-67-2P 117008-24-9P
ROLE: RCT (Reactant); SPN (Synthetic preparation);
PREP (Preparation); RACT (Reactant or reagent)
(preparation and addition reaction of, with nucleophiles)

INDEX TERM: 108162-05-6P 108162-06-7P 116385-36-5P
ROLE: RCT (Reactant); SPN (Synthetic preparation);
PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, with iron complex)

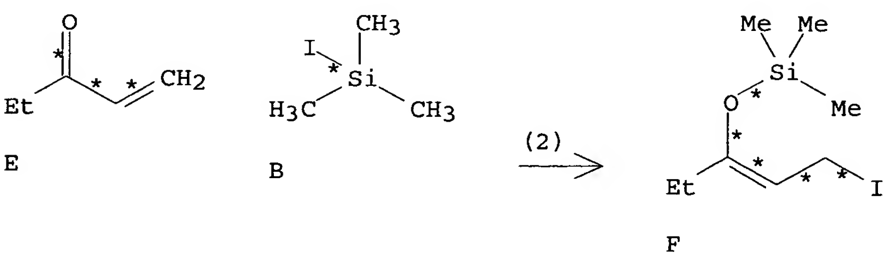
INDEX TERM: 3709-23-7P 5331-68-0P 10407-33-7P 22274-75-5P
70431-98-0P 72357-49-4P 111372-86-2P
116981-00-1P 116981-01-2P 116981-07-8P
116981-08-9P 116981-09-0P 116981-10-3P
116981-11-4P 116994-60-6P
ROLE: SPN (Synthetic preparation); PREP
(Preparation)
(preparation of)

RX(1) OF 50 A + B ===> C...



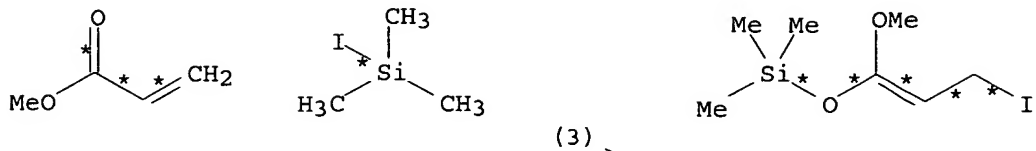
RX(1)	RCT	A 768-03-6, B 16029-98-4
	PRO	C 116385-36-5
	SOL	75-09-2 CH2Cl2

RX(2) OF 50 E + B ===> F...



RX(2)	RCT	E 1629-58-9, B 16029-98-4
	PRO	F 108162-05-6
	SOL	75-09-2 CH2Cl2

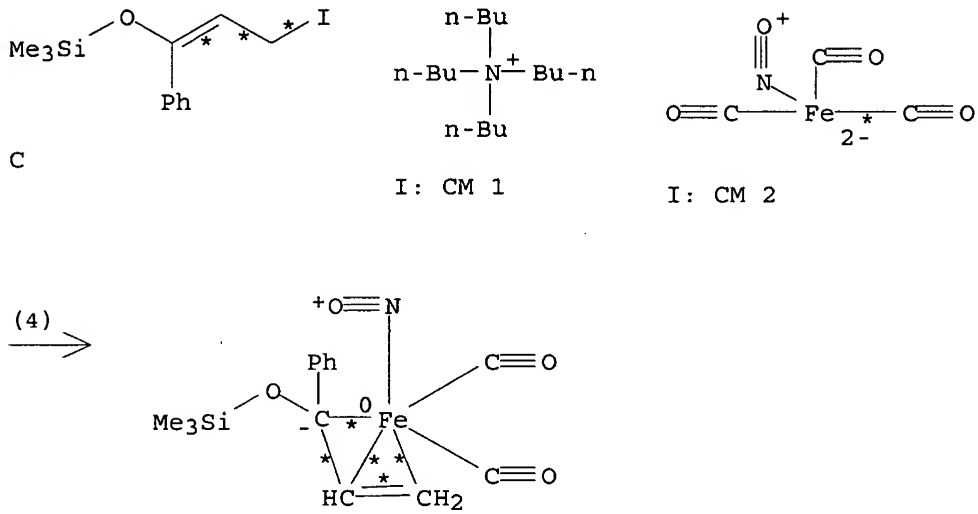
RX(3) OF 50 G + B ===> H...



G B H

RX(3) RCT G 96-33-3, B 16029-98-4
PRO H 108162-06-7
SOL 75-09-2 CH2Cl2

RX(4) OF 50 ...C + I ===> J...

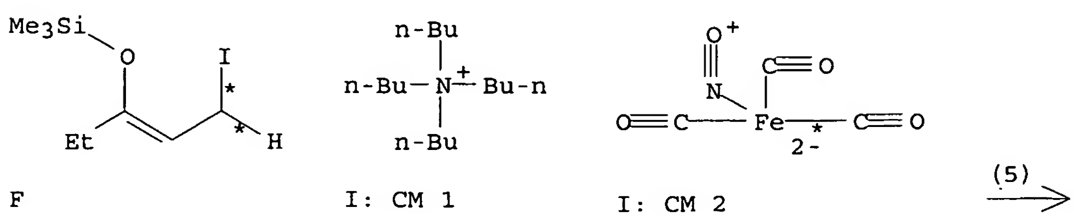


C I: CM 1 I: CM 2

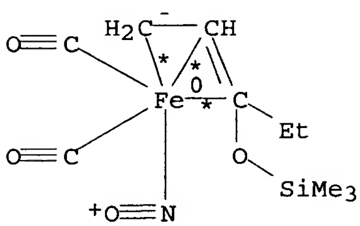
J

RX(4) RCT C 116385-36-5, I 96206-23-4
PRO J 116309-67-2
SOL 75-09-2 CH2Cl2

RX(5) OF 50 ...F + I ===> K...



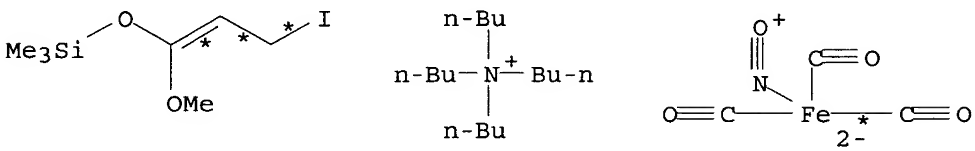
F I: CM 1 I: CM 2



K

RX(5) RCT F 108162-05-6, I 96206-23-4
PRO K 116309-63-8
SOL 75-09-2 CH2Cl2

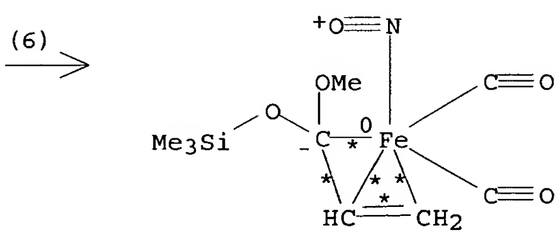
RX(6) OF 50 ...H + I ===> L...



H

I: CM 1

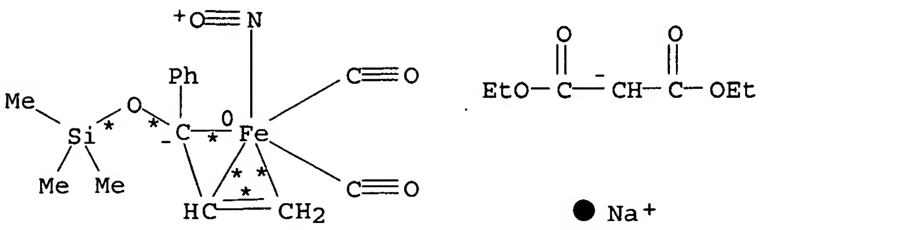
I: CM 2



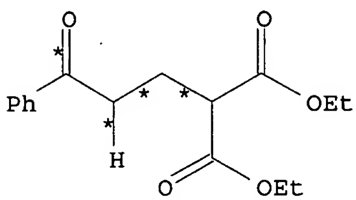
L

RX(6) RCT H 108162-06-7, I 96206-23-4
PRO L 117008-24-9
SOL 75-09-2 CH2Cl2

RX(7) OF 50 ...J + M ===> N



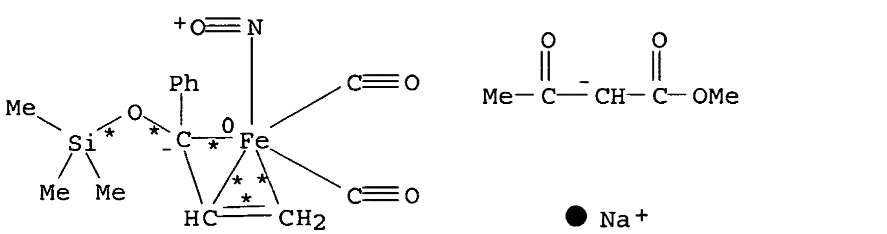
J M



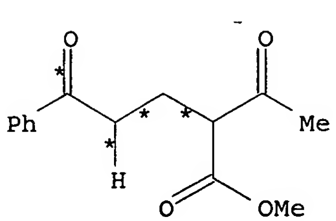
N
YIELD 95%

RX(7) RCT J 116309-67-2, M 996-82-7
PRO N 3709-23-7
SOL 75-09-2 CH2Cl2

RX(8) OF 50 ...J + O ===> P



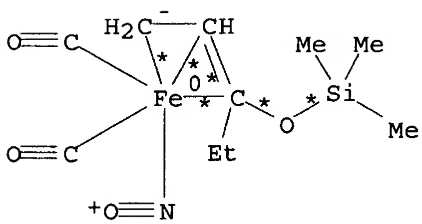
J O



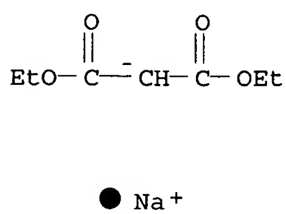
P
YIELD 42%

RX(8) RCT J 116309-67-2, O 34284-28-1
PRO P 116981-00-1
SOL 75-09-2 CH2Cl2

RX(9) OF 50 ...K + M ===> Q

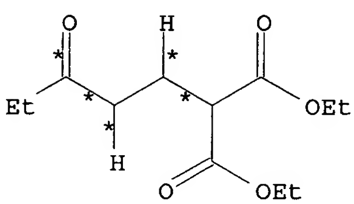


K



M

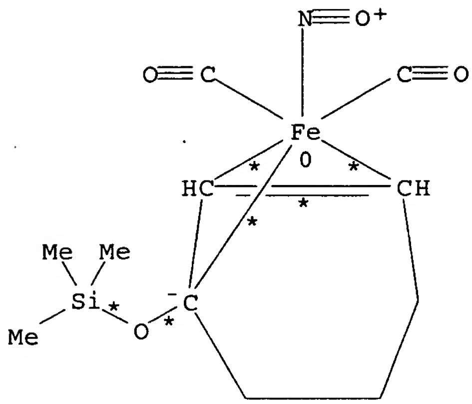
(9) →



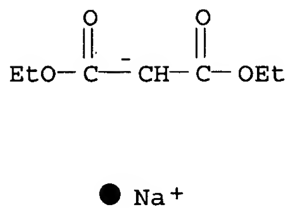
Q
YIELD 75%

RX(9) RCT K 116309-63-8, M 996-82-7
PRO Q 70431-98-0
SOL 75-09-2 CH2Cl2

RX(10) OF 50 R + M ===> S

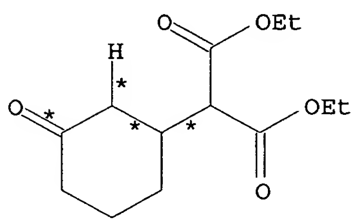


R



M

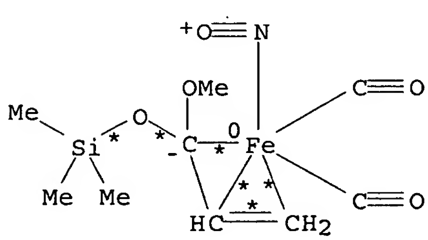
(10) $\longrightarrow$



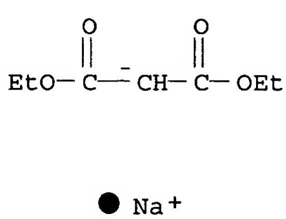
S
YIELD 90%

RX(10) RCT R 116309-64-9, M 996-82-7
PRO S 22274-75-5
SOL 75-09-2 CH2Cl2

RX(11) OF 50 ...L + M ===> T

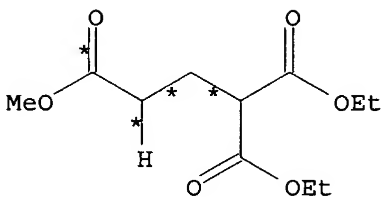


L



M

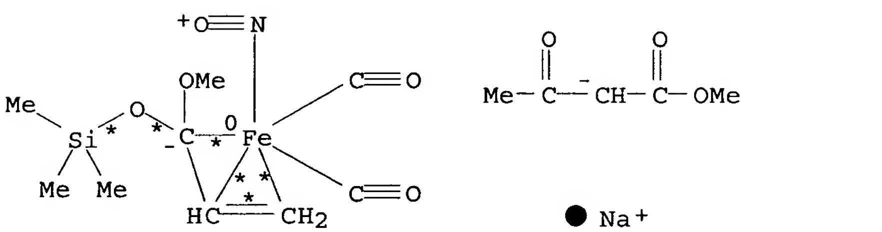
(11) $\longrightarrow$



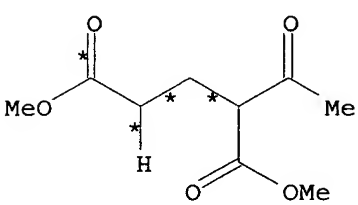
T
YIELD 95%

RX(11) RCT L 117008-24-9, M 996-82-7
PRO T 5331-68-0
SOL 75-09-2 CH2Cl2

RX(12) OF 50 ...L + O ===> U



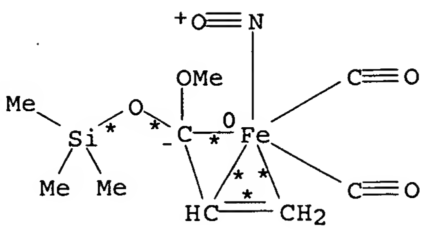
L O



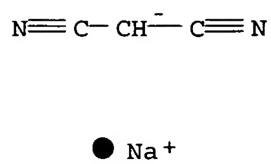
U
YIELD 60%

RX(12) RCT L 117008-24-9, O 34284-28-1
PRO U 116981-01-2
SOL 75-09-2 CH2Cl2

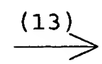
RX(13) OF 50 ...L + V ===> W

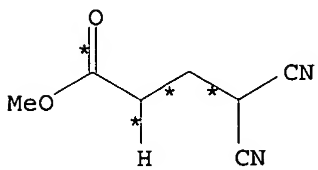


L



V

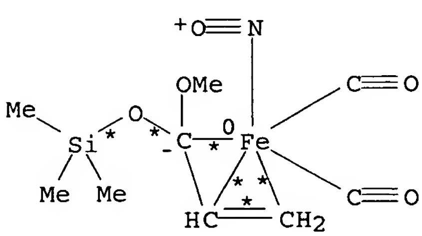




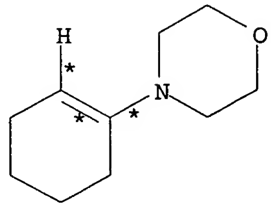
W
YIELD 92%

RX(13) RCT L 117008-24-9, V 20334-42-3
PRO W 111372-86-2
SOL 75-09-2 CH2Cl2

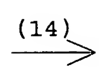
RX(14) OF 50 ...L + X ===> Y

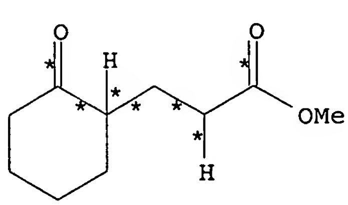


L



X

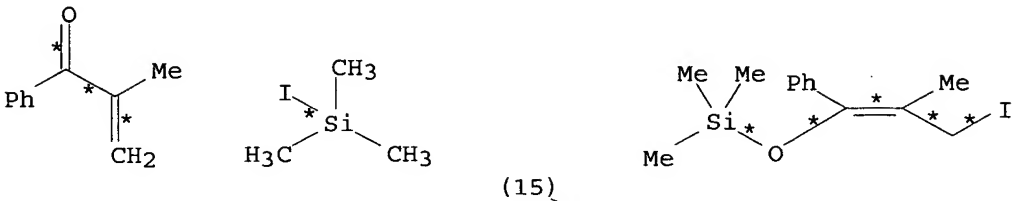




Y
YIELD 89%

RX(14) RCT L 117008-24-9, X 670-80-4
PRO Y 10407-33-7
SOL 75-09-2 CH2Cl2

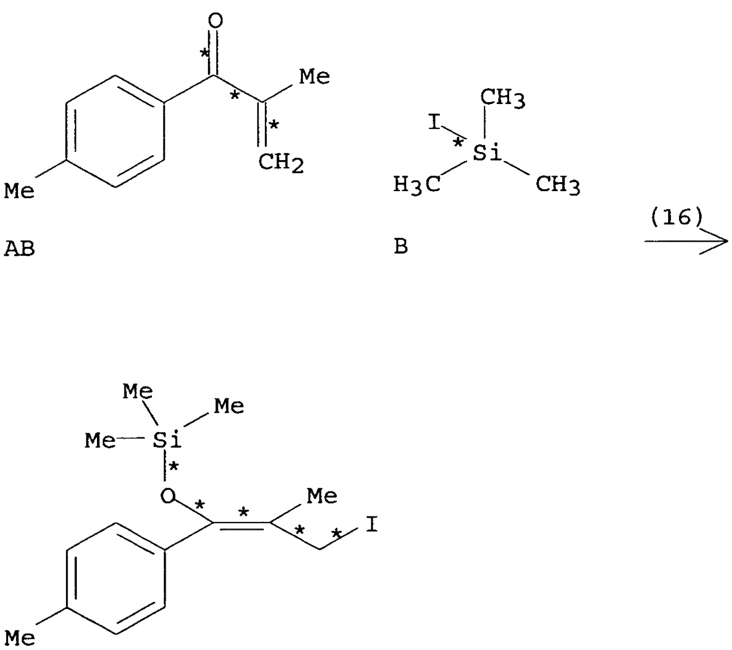
RX(15) OF 50 Z + B ===> AA...



Z B AA

RX(15) RCT Z 769-60-8, B 16029-98-4
PRO AA 116981-02-3
SOL 75-09-2 CH2Cl2

RX(16) OF 50 AB + B ===> AC...

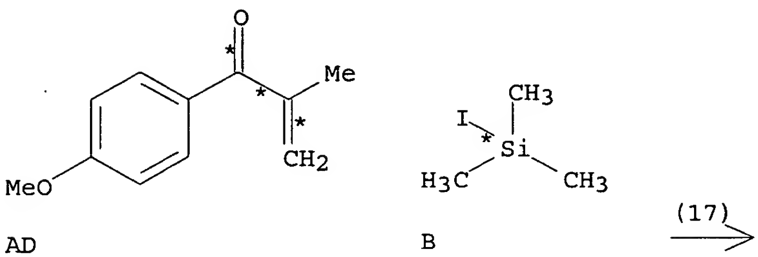


AB B

AC

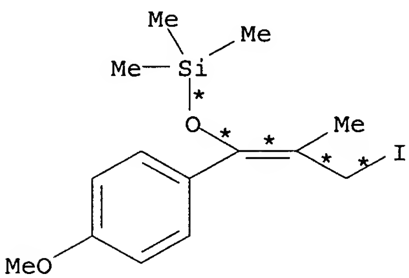
RX(16) RCT AB 62834-89-3, B 16029-98-4
PRO AC 116981-03-4
SOL 75-09-2 CH2Cl2

RX(17) OF 50 AD + B ===> AE...



AD

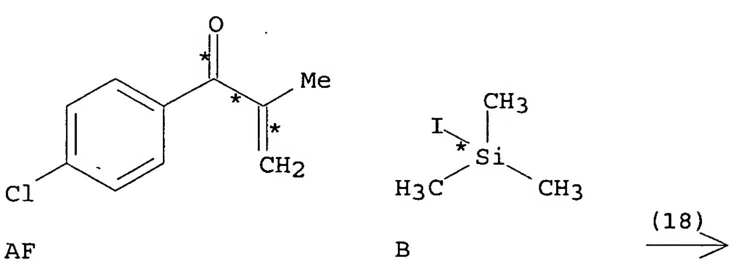
B



AE

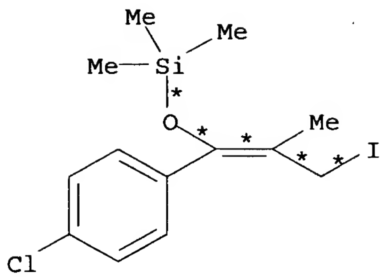
RX(17) RCT AD 6230-72-4, B 16029-98-4
PRO AE 116981-04-5
SOL 75-09-2 CH2Cl2

RX(18) OF 50 AF + B ===> AG...



AF

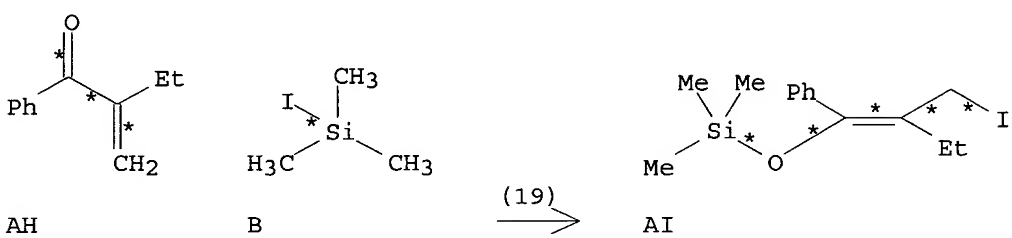
B



AG

RX(18) RCT AF 6230-73-5, B 16029-98-4
PRO AG 116981-05-6
SOL 75-09-2 CH2Cl2

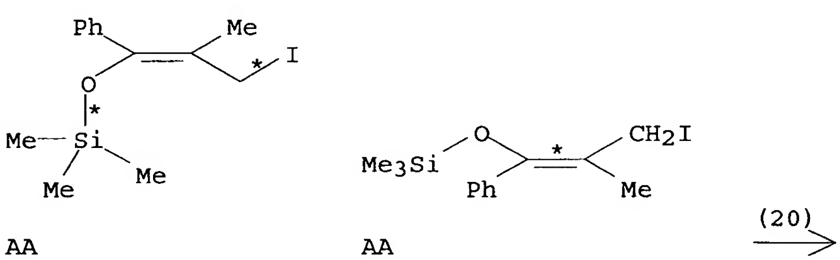
RX(19) OF 50 AH + B ===> AI...



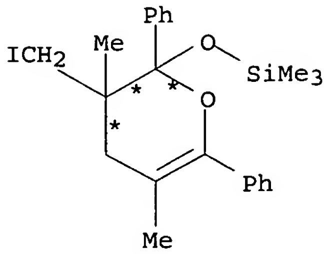
AH B (19) AI

RX(19) RCT AH 22731-65-3, B 16029-98-4
PRO AI 116981-06-7
SOL 75-09-2 CH2Cl2

RX(20) OF 50 ...2 AA ===> AJ



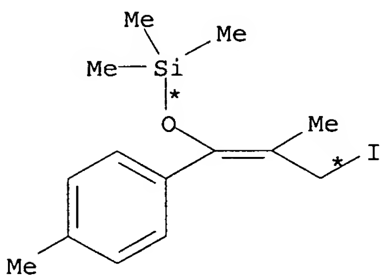
AA AA (20)



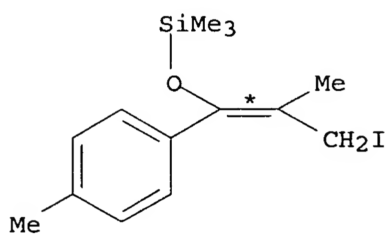
AJ

RX(20)	RCT	AA 116981-02-3
	RGT	I 96206-23-4 1-Butanaminium, N,N,N-tributyl-, (T-4)-tricarbonylnitrosylferrate(1-)
	PRO	AJ 116981-07-8
	SOL	75-09-2 CH2Cl2

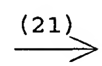
RX(21) OF 50 ...2 AC ===> AK

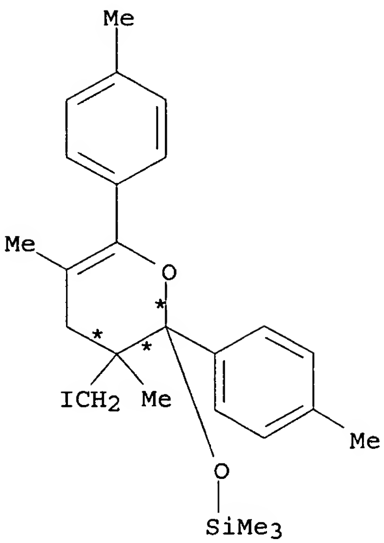


AC



AC

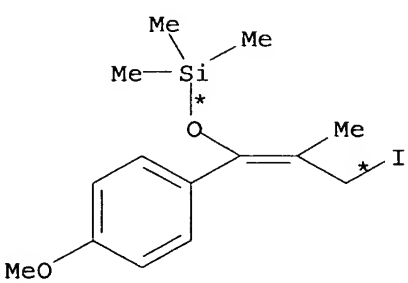




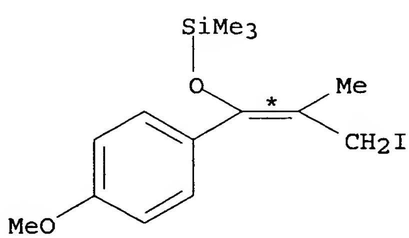
AK

RX(21) RCT AC 116981-03-4
RGT I 96206-23-4 1-Butanaminium, N,N,N-tributyl-, (T-4)-tricarbonylnitrosylferrate(1-)
PRO AK 116981-08-9
SOL 75-09-2 CH2Cl2

RX(22) OF 50 ...2 AE ===> AL

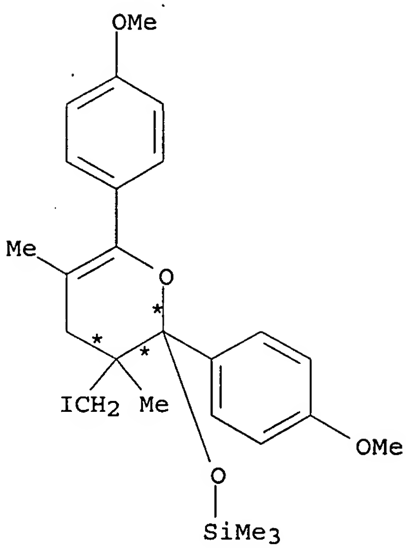


AE



AE

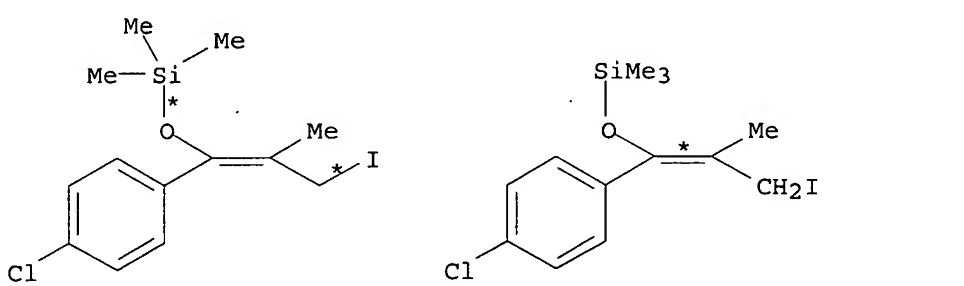
(22) →



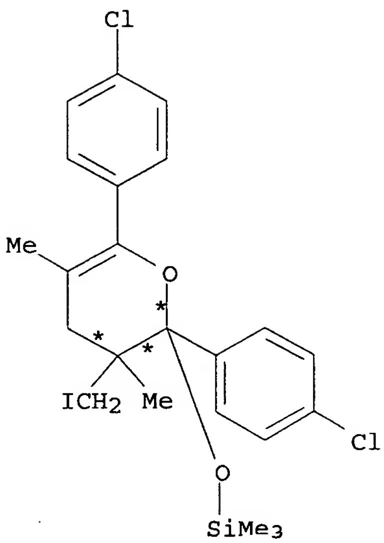
AL

RX(22) RCT AE 116981-04-5
RGT I 96206-23-4 1-Butanaminium, N,N,N-tributyl-, (T-4)-tricarbonylnitrosylferrate(1-)
PRO AL 116981-09-0
SOL 75-09-2 CH2Cl2

RX(23) OF 50 ...2 AG ===> AM



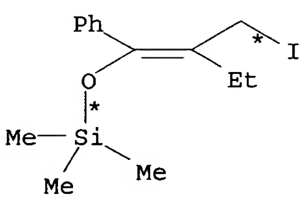
AG AG



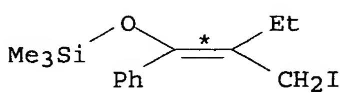
AM

RX(23) RCT AG 116981-05-6
RGT I 96206-23-4 1-Butanaminium, N,N,N-tributyl-, (T-4)-tricarbonylnitrosylferrate(1-)
PRO AM 116981-10-3
SOL 75-09-2 CH2Cl2

RX(24) OF 50 ...2 AI ===> AN

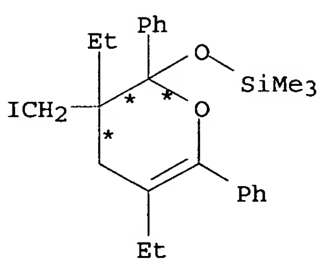


AI



AI

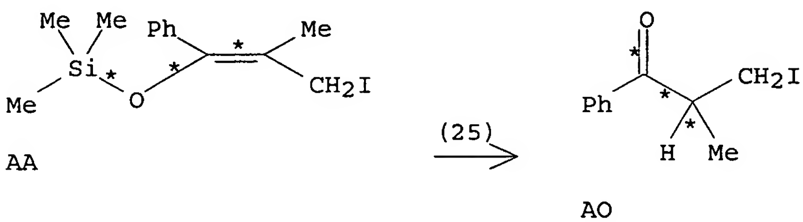
$\xrightarrow{(24)}$



AN

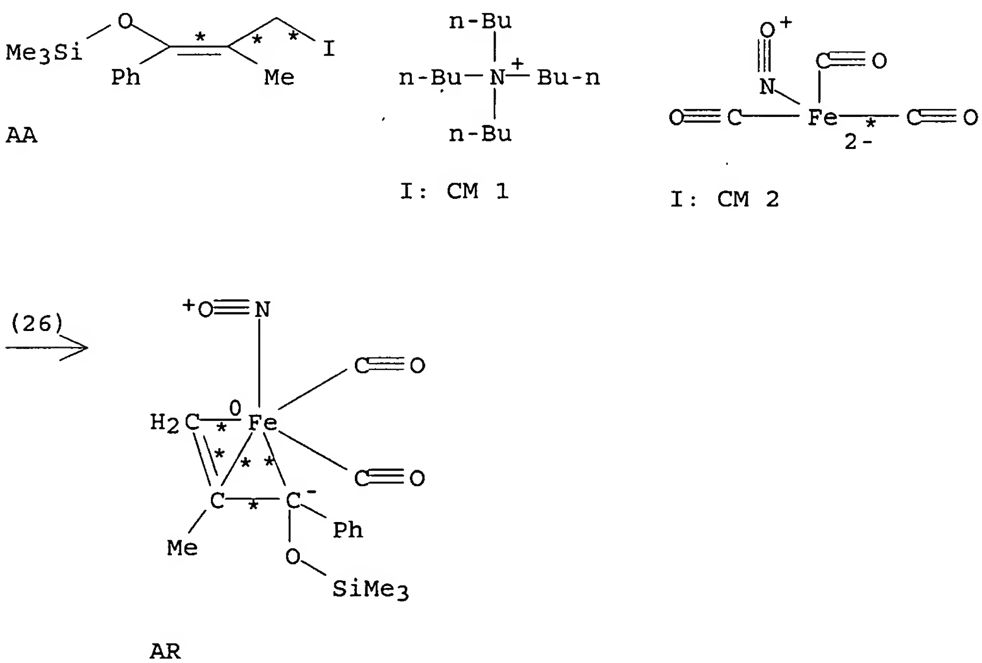
RX(24) RCT AI 116981-06-7
RGT I 96206-23-4 1-Butanaminium, N,N,N-tributyl-, (T-4)-tricarbonylnitrosylferrate(1-)
PRO AN 116981-11-4
SOL 75-09-2 CH2Cl2

RX(25) OF 50 ...AA ===> AO



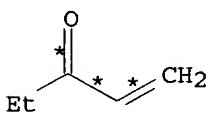
RX(25) RCT AA 116981-02-3
RGT AP 7647-01-0 HCl
PRO AO 72357-49-4
SOL 7732-18-5 Water

RX(26) OF 50 ...AA + I ===> AR

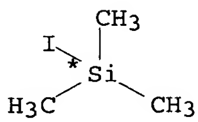


RX(26) RCT AA 116981-02-3, I 96206-23-4
PRO AR 116994-60-6
SOL 75-09-2 CH2Cl2

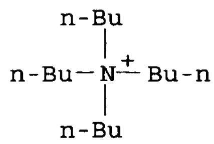
RX(46) OF 50 COMPOSED OF RX(2), RX(5), RX(9)
RX(46) **E** + B + **I** + **M** ===>
Q



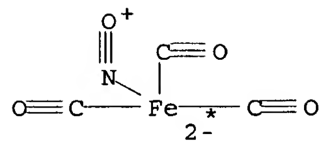
E



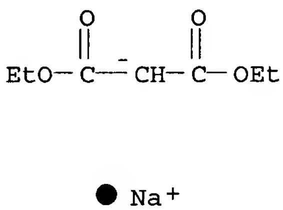
B



I: CM 1

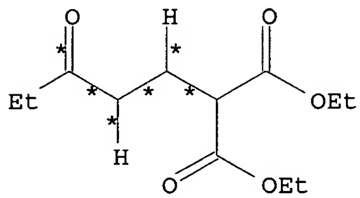


I: CM 2



M

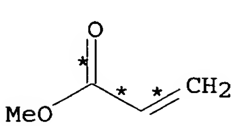
3
STEPS



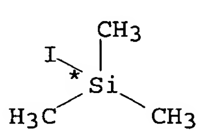
Q
YIELD 75%

RX(2)	RCT	E **1629-58-9**, B 16029-98-4
	PRO	F 108162-05-6
	SOL	75-09-2 CH2Cl2
RX(5)	RCT	F 108162-05-6, I **96206-23-4**
	PRO	K 116309-63-8
	SOL	75-09-2 CH2Cl2
RX(9)	RCT	K 116309-63-8, M **996-82-7**
	PRO	Q **70431-98-0**
	SOL	75-09-2 CH2Cl2

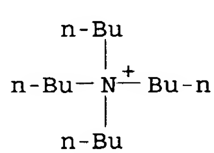
RX(47) OF 50 COMPOSED OF RX(3), RX(6), RX(11)
RX(47) **G** + B + **I** + **M** ===>
T



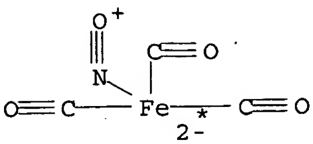
G



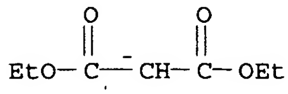
B



I: CM 1



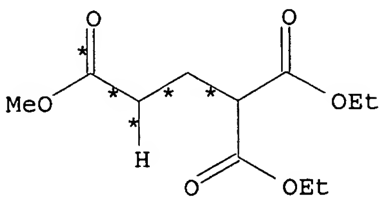
I: CM 2



● Na+

M

3 STEPS →



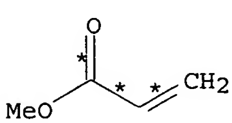
T
YIELD 95%

RX(3) RCT G **96-33-3**, B 16029-98-4
PRO H 108162-06-7
SOL 75-09-2 CH2Cl2

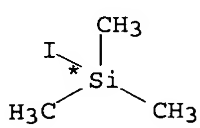
RX(6) RCT H 108162-06-7, I **96206-23-4**
PRO L 117008-24-9
SOL 75-09-2 CH2Cl2

RX(11) RCT L 117008-24-9, M **996-82-7**
PRO T **5331-68-0**
SOL 75-09-2 CH2Cl2

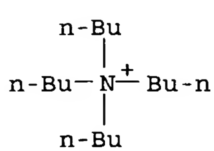
RX(48) OF 50 COMPOSED OF RX(3), RX(6), RX(12)
RX(48) **G** + B + **I** + **O** ===>
U



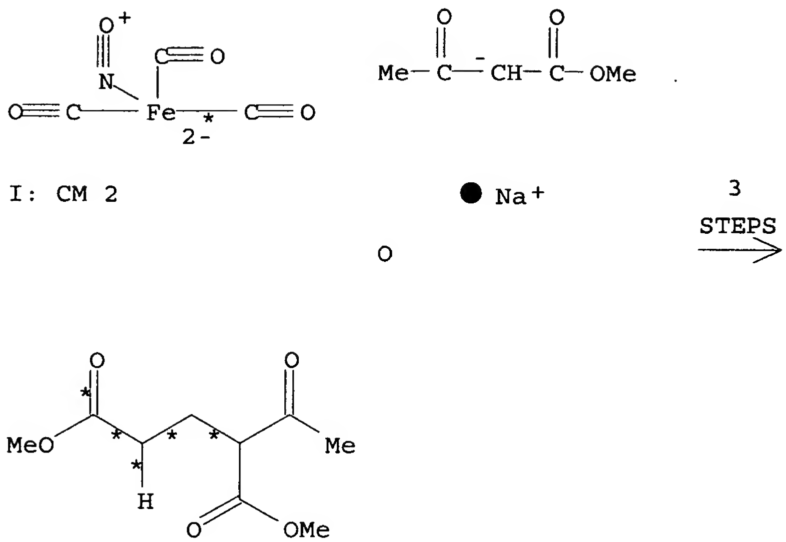
G



B



I: CM 1



YIELD 60%

```
RX(3)      RCT  G 96-33-3, B 16029-98-4
           PRO  H 108162-06-7
           SOL  75-09-2 CH2Cl2

RX(6)      RCT  H 108162-06-7, I 96206-23-4
           PRO  L 117008-24-9
           SOL  75-09-2 CH2Cl2

RX(12)     RCT  L 117008-24-9, O 34284-28-1
           PRO  U 116981-01-2
           SOL  75-09-2 CH2Cl2
```

L20 ANSWER 7 OF 7 CASREACT

ACCESSION NUMBER: 106:137899 CASREACT

TITLE: Synthesis of functionalized 1,4-dienes by addition of functionalized allylzinc compounds to alkynes and their cyclization to heterocycles and carbocycles

AUTHOR(S): Knochel, P.; Normant, J. F.
CORPORATE SOURCE: Lab. Chim. Org. Elem., Univ. P. M. Curie, Paris, 75230/05, Fr.

SOURCE: Journal of Organometallic Chemistry (1986), 309(1-2), 1-23
CODEN: JORCAI; ISSN: 0022-328X
DOCUMENT TYPE: Journal
LANGUAGE: French
CLASSIFICATION: 23-3 (Aliphatic Compounds)
Section cross-reference(s): 27, 28

ABSTRACT:

The regiospecific addition of functionalized allylic bromides to terminal alkynes in the presence of zinc furnishes a great variety of highly functionalized 1,4-dienes with moderate to good yields. The synthetic utility of these 1,4-dienes is demonstrated by various cyclization

reactions leading to an α-methylene-γ-butyrolactone, to 3,5-difunctionalized piperidines, to a cyclic triester and to 6- or 7-membered phosphorus heterocyclic compds.

SUPPL. TERM: allyl bromide addn alkyne zinc; piperidine; oxaphosphorinane oxo alkoxy

INDEX TERM: Allylic compounds
ROLE: RCT (Reactant); RACT (Reactant or reagent)
(bromides, functionalized, addition reaction of, with terminal alkynes and zinc)

INDEX TERM: Addition reaction
(of functionalized allyl bromides with terminal alkynes and zinc)

INDEX TERM: Alkynes
ROLE: RCT (Reactant); RACT (Reactant or reagent)
(α-, addition reaction of, with functionalized allyl bromides and zinc)

INDEX TERM: 122-52-1, Triethyl phosphite
ROLE: RCT (Reactant); RACT (Reactant or reagent)
(Arbuzov reaction of, with methylene bromide)

INDEX TERM: 74-95-3, Methylene bromide
ROLE: RCT (Reactant); RACT (Reactant or reagent)
(Arbuzov reaction of, with tri-Et phosphite)

INDEX TERM: 75-36-5, Acetyl chloride
ROLE: RCT (Reactant); RACT (Reactant or reagent)
(acylation by, of allyl silyl ethers)

INDEX TERM: 627-09-8 629-05-0, 1-Octyne 5651-88-7, Phenyl propargyl sulfide 13361-64-3, Propargyltrimethylsilane 13397-78-9 17869-76-0 18938-38-0
ROLE: RCT (Reactant); RACT (Reactant or reagent)
(addition reaction of, with functionalized allyl bromide derivative and zinc)

INDEX TERM: 693-02-7, 1-Hexyne 5582-62-7, Propargyl trimethylsilyl ether 16314-18-4 17869-75-9
ROLE: RCT (Reactant); RACT (Reactant or reagent)
(addition reaction of, with functionalized allyl bromides and zinc)

INDEX TERM: 62097-05-6
ROLE: RCT (Reactant); RACT (Reactant or reagent)
(addition reaction of, with propargyl silyl ether derivative and zinc)

INDEX TERM: 123-75-1, Pyrrolidine, reactions
ROLE: RCT (Reactant); RACT (Reactant or reagent)
(amidation by, of dibromoisobutyric acid)

INDEX TERM: 63164-16-9
ROLE: RCT (Reactant); RACT (Reactant or reagent)
(amidation of, by pyrrolidine)

INDEX TERM: 38281-98-0
ROLE: RCT (Reactant); RACT (Reactant or reagent)
(bromination of)

INDEX TERM: 55287-89-3
ROLE: PROC (Process)
(conversion of, to allyl bromide analog)

INDEX TERM: 37850-75-2
ROLE: RCT (Reactant); RACT (Reactant or reagent)
(conversion of, to dibromoisopropyl sulfoxide derivative)

INDEX TERM: 111-68-2, 1-Heptylamine
ROLE: RCT (Reactant); RACT (Reactant or reagent)

(cycloaddn. reaction of, with pentadiene derivative)
INDEX TERM: 100-46-9, Benzylamine, reactions
ROLE: RCT (Reactant); RACT (Reactant or reagent)
(cycloaddn. reaction of, with pentadienes)
INDEX TERM: 105-53-3, Diethyl malonate
ROLE: RCT (Reactant); RACT (Reactant or reagent)
(cycloaddn.-cyclocondensation of, with pentenyl acetate derivative)
INDEX TERM: 115-11-7, Isobutylene, reactions
ROLE: RCT (Reactant); RACT (Reactant or reagent)
(esterification by, of bromoacetic acid)
INDEX TERM: 79-08-3, Bromoacetic acid
ROLE: RCT (Reactant); RACT (Reactant or reagent)
(esterification of)
INDEX TERM: 107345-39-1P
ROLE: FORM (Formation, nonpreparative); PREP (Preparation)
(formation of, in addition reaction of carbalkoxyallyl bromide with alkynes and zinc)
INDEX TERM: 107345-41-5P
ROLE: FORM (Formation, nonpreparative); PREP (Preparation)
(formation of, in attempted addition reaction of allyl bromide derivative with hexyne and zinc)
INDEX TERM: 1125-99-1
ROLE: RCT (Reactant); RACT (Reactant or reagent)
(hydrolysis of, and alkylation of product with pentenyl acetate derivative)
INDEX TERM: 91476-12-9P
ROLE: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and acetylation of)
INDEX TERM: 107345-23-3P 107345-24-4P
ROLE: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and addition reaction of, with propargyl silyl ether derivative and zinc)
INDEX TERM: 17435-72-2P 53913-96-5P 84308-48-5P 91445-18-0P 91476-10-7P 97147-24-5P
ROLE: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and addition reaction of, with terminal alkynes and zinc)
INDEX TERM: 1660-94-2P
ROLE: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and conversion, to isopropenylphosphonic acid derivative)
INDEX TERM: 91476-26-5P
ROLE: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and cycloaddn. reaction of, with amines)
INDEX TERM: 107345-42-6P
ROLE: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and cycloaddn. reaction of, with benzylamine)
INDEX TERM: 91476-21-0P 91476-22-1P 91476-23-2P 91476-24-3P
ROLE: RCT (Reactant); SPN (Synthetic preparation);

PREP (Preparation); RACT (Reactant or reagent)
(preparation and cyclocondensation reaction of)

INDEX TERM: 5292-43-3P, 1,1-Dimethylethyl bromoacetate
ROLE: SPN (Synthetic preparation); PREP (Preparation)
(preparation and cyclocondensation with alkyne and zinc)

INDEX TERM: 107345-37-9P 107345-38-0P
ROLE: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and dehydrobromination of)

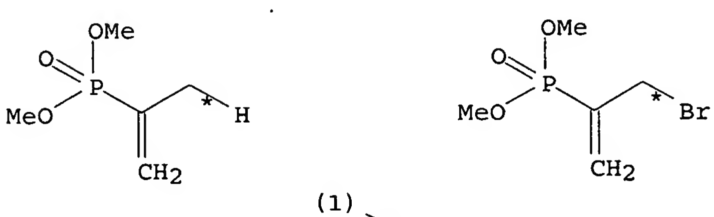
INDEX TERM: 91476-11-8P
ROLE: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and iodolactonization of)

INDEX TERM: 93032-43-0P
ROLE: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, with phosphorus tribromide)

INDEX TERM: 91476-13-0P 91476-14-1P 91476-15-2P
91476-16-3P 91476-17-4P 91476-18-5P
91476-19-6P 91476-20-9P 91476-25-4P
91476-27-6P 91476-28-7P 91476-29-8P
91476-30-1P 91476-31-2P 91476-32-3P
91476-33-4P 94225-07-7P 94225-08-8P
94225-09-9P 97779-25-4P 97779-26-5P
97779-27-6P 107345-25-5P 107345-26-6P
107345-27-7P 107345-28-8P 107345-29-9P
107345-30-2P 107345-31-3P 107345-32-4P
107345-33-5P 107345-34-6P 107345-35-7P
107345-36-8P 107345-40-4P 107345-43-7P
107345-44-8P 107345-45-9P
ROLE: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

INDEX TERM: 50-00-0, Formaldehyde, reactions
ROLE: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with methylenebisphosphonic acid derivative)

RX(1) OF 130 A ===> B...



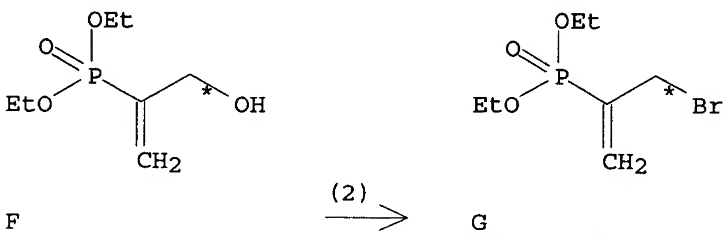
A

B
YIELD 37%

RX(1) RCT A 38281-98-0
RGT C 128-08-5 Bromosuccinimide, D 78-67-1 AIBN
PRO B 84308-48-5

SOL 56-23-5 CCl4

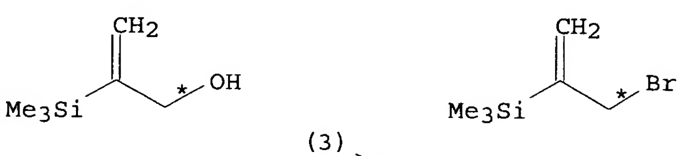
RX(2) OF 130 ...F ===> G...



F (2) → G
YIELD 56%

RX(2) RCT F 93032-43-0
RGT H 7789-60-8 PBr3
PRO G 91476-10-7
SOL 60-29-7 Et2O

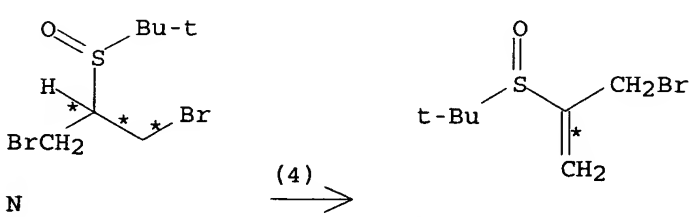
RX(3) OF 130 J ===> K...



J (3) → K
YIELD 63%

RX(3) RCT J 55287-89-3
RGT C 128-08-5 Bromosuccinimide, L 75-18-3 Me2S
PRO K 91445-18-0
SOL 75-09-2 CH2Cl2

RX(4) OF 130 ...N ===> O...

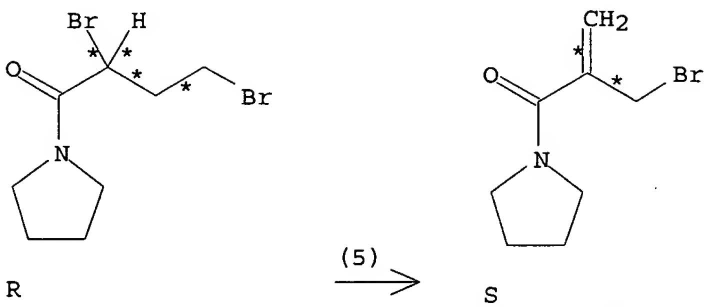


N (4) → O
YIELD 74%

RX(4) RCT N 107345-37-9
RGT P 6674-22-2 DBU, Q 123-31-9 Hydroquinone

PRO O 107345-23-3
SOL 75-09-2 CH2Cl2

RX(5) OF 130 ...R ===> S...

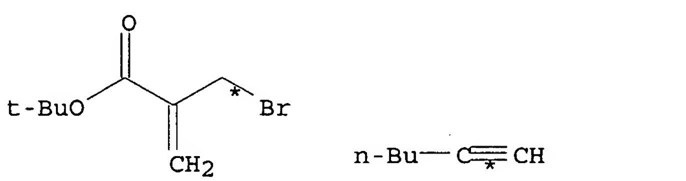


R

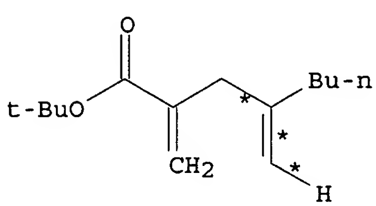
S
YIELD 67%

RX(5) RCT R 107345-38-0
RGT P 6674-22-2 DBU, Q 123-31-9 Hydroquinone
PRO S 107345-24-4
SOL 75-09-2 CH2Cl2

RX(6) OF 130 T + U ===> V...



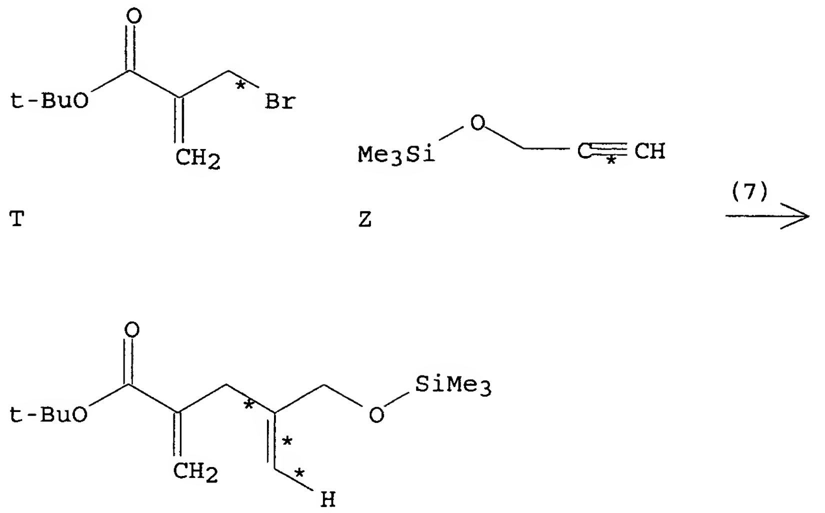
T U



V
YIELD 70%

RX(6) RCT T 53913-96-5, U 693-02-7
RGT W 7440-66-6 Zn, X 106-93-4 BrCH2CH2Br
PRO V 91476-11-8
SOL 109-99-9 THF

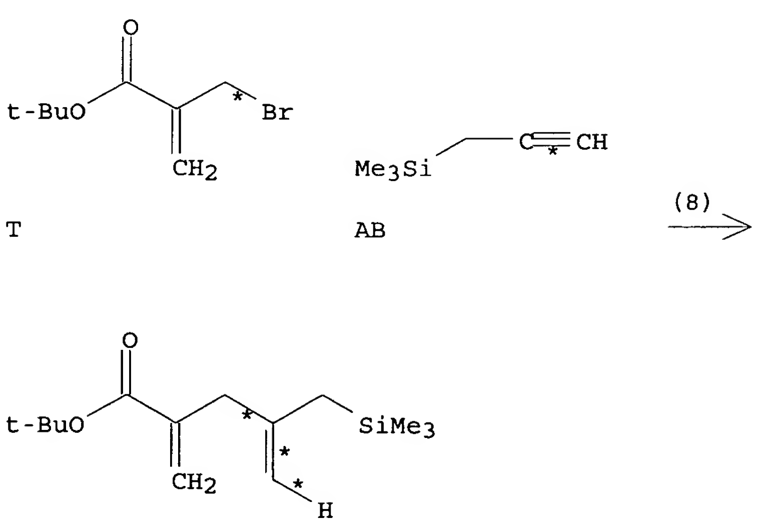
RX(7) OF 130 T + Z ===> AA...



AA
YIELD 81%

RX(7) RCT T 53913-96-5, Z 5582-62-7
RGT W 7440-66-6 Zn, X 106-93-4 BrCH2CH2Br
PRO AA 91476-12-9
SOL 109-99-9 THF

RX(8) OF 130 T + AB ===> AC

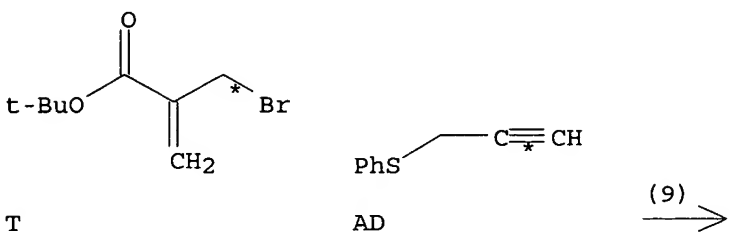


AC
YIELD 24%

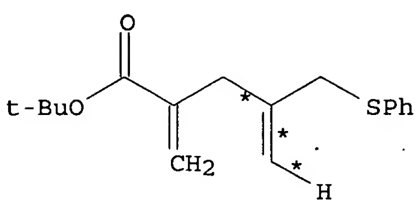
RX(8) RCT T 53913-96-5, AB 13361-64-3

RGT W 7440-66-6 Zn, X 106-93-4 BrCH2CH2Br
PRO AC 107345-25-5
SOL 109-99-9 THF

RX(9) OF 130 T + AD ===> AE



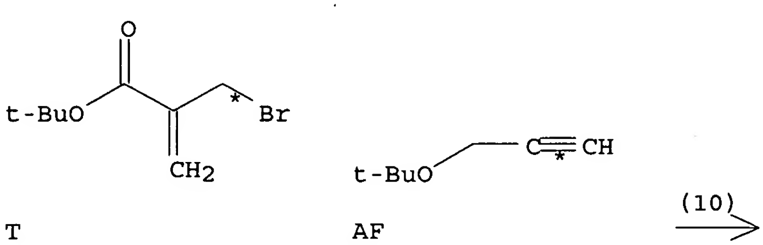
T AD



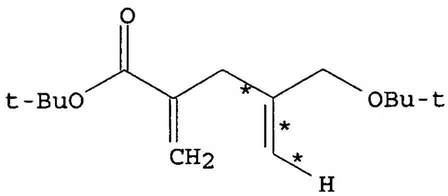
AE
YIELD 55%

RX(9) RCT T 53913-96-5, AD 5651-88-7
RGT W 7440-66-6 Zn, X 106-93-4 BrCH2CH2Br
PRO AE 91476-16-3
SOL 109-99-9 THF

RX(10) OF 130 T + AF ===> AG



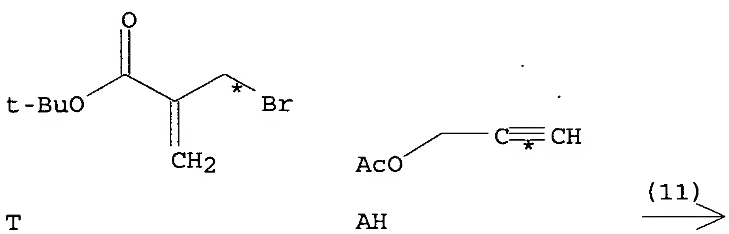
T AF



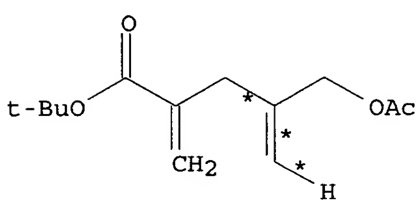
AG
YIELD 64%

RX(10) RCT T 53913-96-5, AF 16314-18-4
RGT W 7440-66-6 Zn, X 106-93-4 BrCH2CH2Br
PRO AG 91476-14-1
SOL 109-99-9 THF

RX(11) OF 130 T + AH ===> AI...



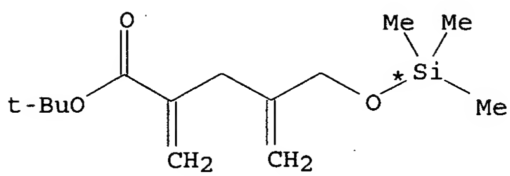
T AH



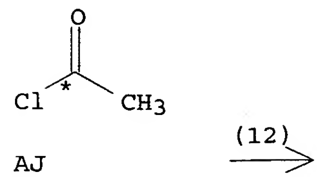
AI
YIELD 47%

RX(11) RCT T 53913-96-5, AH 627-09-8
RGT W 7440-66-6 Zn, X 106-93-4 BrCH2CH2Br
PRO AI 91476-26-5
SOL 109-99-9 THF

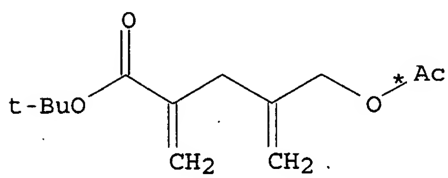
RX(12) OF 130 ...AA + AJ ===> AI...



AA



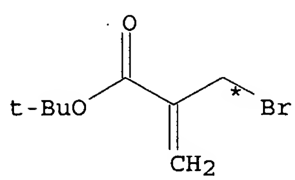
AJ



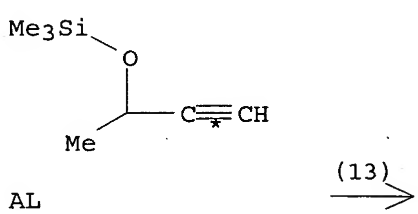
AI
YIELD 88%

```
RX(12)     RCT  AA 91476-12-9, AJ 75-36-5
           RGT  AK 64-19-7 AcOH
           PRO  AI 91476-26-5
           SOL  60-29-7 Et2O, 64-19-7 AcOH
```

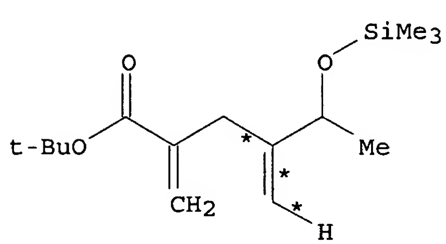
RX(13) OF 130   T + AL ===> AM



T



AL

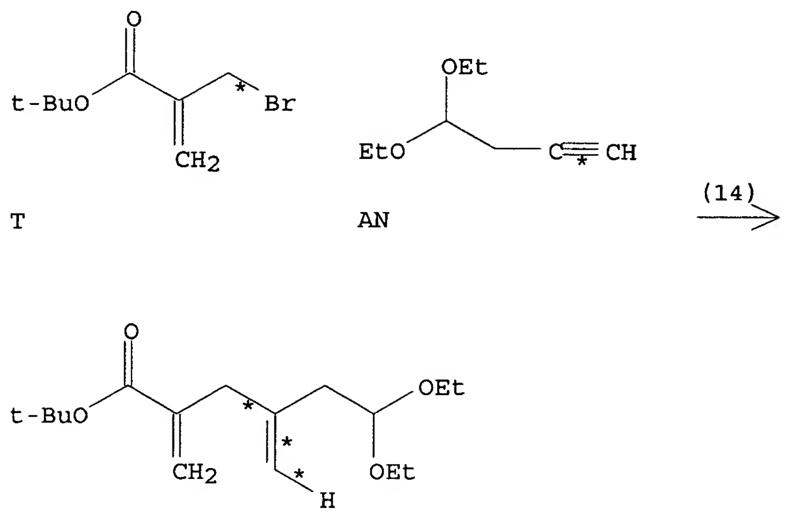


AM
YIELD 54%

```
RX(13)     RCT  T 53913-96-5, AL 17869-76-0
           RGT  W 7440-66-6 Zn, X 106-93-4 BrCH2CH2Br
```

PRO AM 91476-15-2
SOL 109-99-9 THF

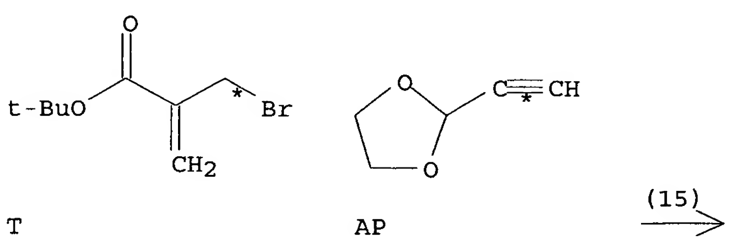
RX(14) OF 130 T + AN ===> AO

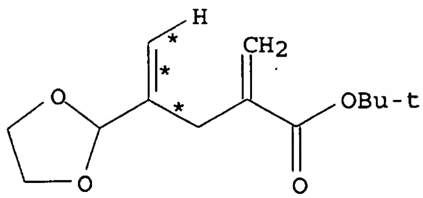


AO
YIELD 60%

RX(14) RCT T 53913-96-5, AN 13397-78-9
RGT W 7440-66-6 Zn, X 106-93-4 BrCH2CH2Br
PRO AO 91476-17-4
SOL 109-99-9 THF

RX(15) OF 130 T + AP ===> AQ

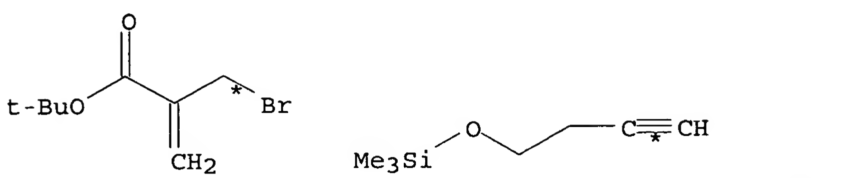




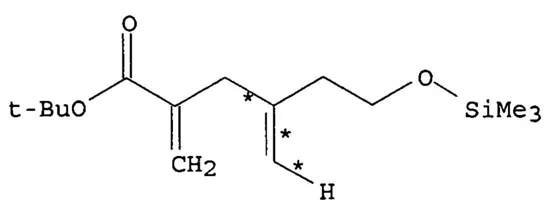
AQ
YIELD 28%

RX(15) RCT T 53913-96-5, AP 18938-38-0
RGT W 7440-66-6 Zn, X 106-93-4 BrCH2CH2Br
PRO AQ 107345-26-6
SOL 109-99-9 THF

RX(16) OF 130 T + AR ===> AS



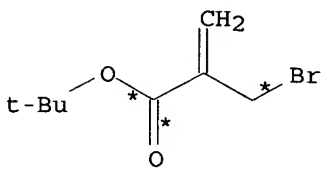
T AR



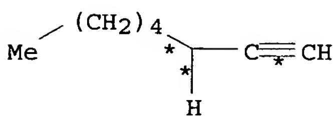
AS
YIELD 70%

RX(16) RCT T 53913-96-5, AR 17869-75-9
RGT W 7440-66-6 Zn, X 106-93-4 BrCH2CH2Br
PRO AS 91476-13-0
SOL 109-99-9 THF

RX(17) OF 130 T + AT ===> AU

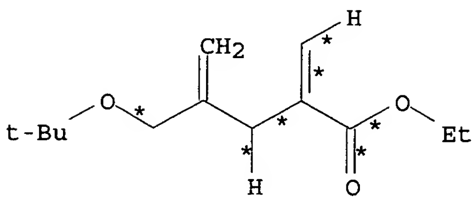


T



AT

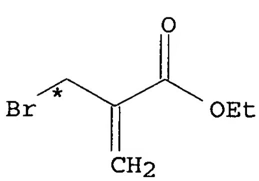
(17)
→



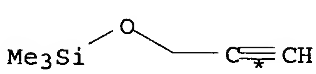
AU
YIELD 62%

RX(17) RCT T 53913-96-5, AT 629-05-0
RGT W 7440-66-6 Zn, X 106-93-4 BrCH2CH2Br
PRO AU 91476-18-5
SOL 109-99-9 THF

RX(18) OF 130 AV + Z ===> AW

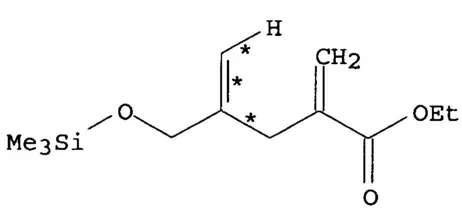


AV



Z

(18)
→

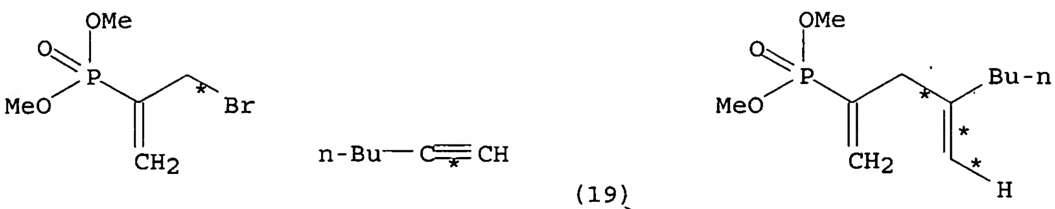


AW
YIELD 68%

RX(18) RCT AV 17435-72-2, Z 5582-62-7
RGT W 7440-66-6 Zn, X 106-93-4 BrCH2CH2Br
PRO AW 91476-19-6

SOL 109-99-9 THF

RX(19) OF 130 ...B + U ===> AX

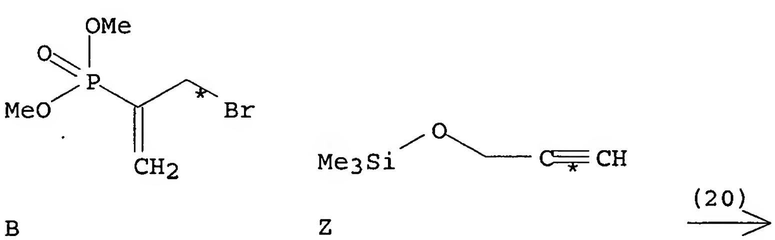


B U AX

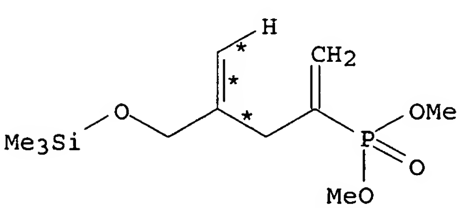
YIELD 48%

RX(19) RCT B 84308-48-5, U 693-02-7
RGT W 7440-66-6 Zn, X 106-93-4 BrCH2CH2Br
PRO AX 91476-20-9
SOL 109-99-9 THF

RX(20) OF 130 ...B + Z ===> AY...



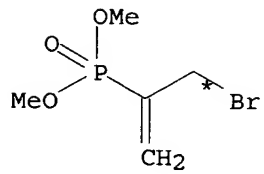
B Z



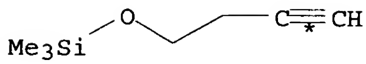
AY

RX(20) RCT B 84308-48-5, Z 5582-62-7
RGT W 7440-66-6 Zn, X 106-93-4 BrCH2CH2Br
PRO AY 107345-27-7
SOL 109-99-9 THF

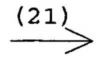
RX(21) OF 130 ...B + AR ===> AZ...

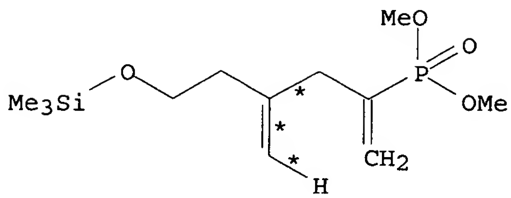


B



AR

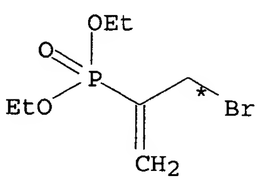




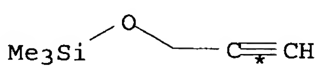
AZ

RX(21) RCT B 84308-48-5, AR 17869-75-9
RGT W 7440-66-6 Zn, X 106-93-4 BrCH2CH2Br
PRO AZ 107345-28-8
SOL 109-99-9 THF

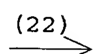
RX(22) OF 130 ...G + Z ===> BA...

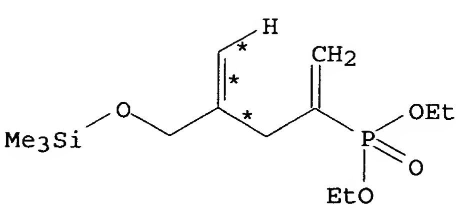


G



Z

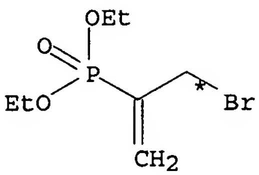




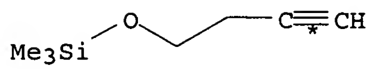
BA

RX(22) RCT G 91476-10-7, Z 5582-62-7
RGT W 7440-66-6 Zn, X 106-93-4 BrCH2CH2Br
PRO BA 107345-29-9
SOL 109-99-9 THF

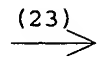
RX(23) OF 130 ...G + AR ===> BB...

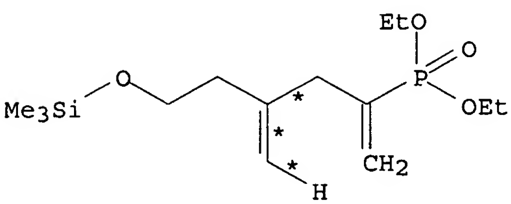


G



AR

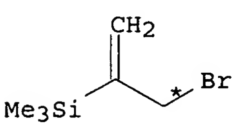




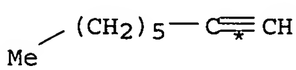
BB

RX(23) RCT G 91476-10-7, AR 17869-75-9
RGT W 7440-66-6 Zn, X 106-93-4 BrCH2CH2Br
PRO BB 107345-30-2
SOL 109-99-9 THF

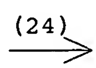
RX(24) OF 130 ...K + AT ===> BC

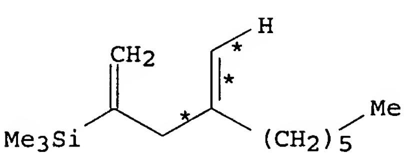


K



AT

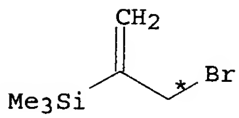




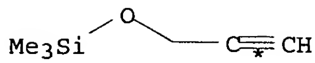
BC
YIELD 50%

RX(24) RCT K 91445-18-0, AT 629-05-0
RGT W 7440-66-6 Zn, X 106-93-4 BrCH2CH2Br
PRO BC 94225-07-7
SOL 109-99-9 THF

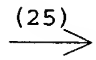
RX(25) OF 130 ...K + Z ===> BD

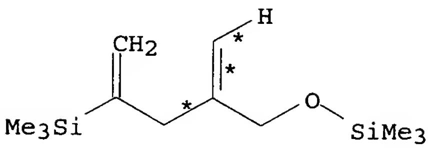


K



Z

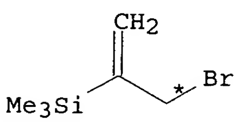




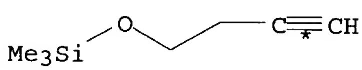
BD
YIELD 60%

RX(25) RCT K 91445-18-0, Z 5582-62-7
RGT W 7440-66-6 Zn, X 106-93-4 BrCH2CH2Br
PRO BD 94225-08-8
SOL 109-99-9 THF

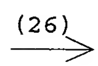
RX(26) OF 130 ...K + AR ===> BE

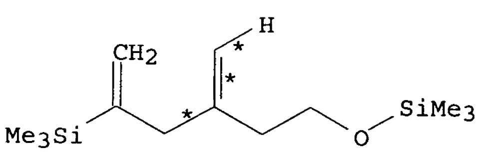


K



AR

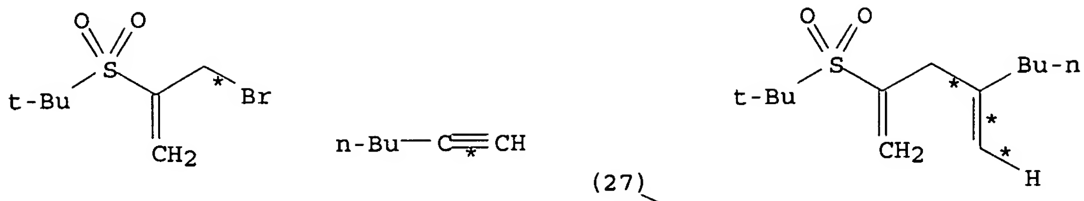




BE
YIELD 60%

RX(26) RCT K 91445-18-0, AR 17869-75-9
RGT W 7440-66-6 Zn, X 106-93-4 BrCH2CH2Br
PRO BE 94225-09-9
SOL 109-99-9 THF

RX(27) OF 130 BF + U ===> BG

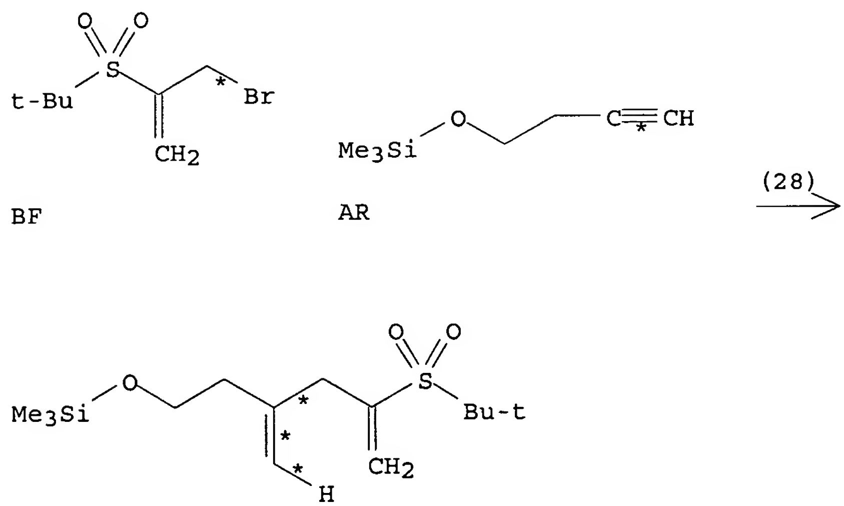


BF U

BG
YIELD 20%

RX(27) RCT BF 97147-24-5, U 693-02-7
RGT W 7440-66-6 Zn, X 106-93-4 BrCH2CH2Br
PRO BG 97779-27-6
SOL 109-99-9 THF

RX(28) OF 130 BF + AR ===> BH...

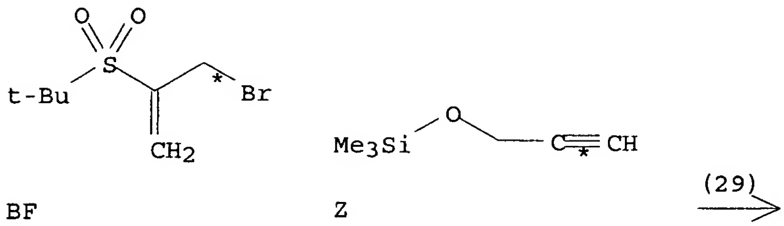


BF AR

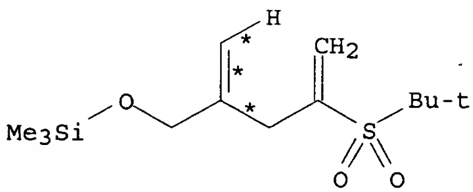
BH

RX(28) RCT BF 97147-24-5, AR 17869-75-9
RGT W 7440-66-6 Zn, X 106-93-4 BrCH2CH2Br
PRO BH 107345-31-3
SOL 109-99-9 THF

RX(29) OF 130 BF + Z ===> BI...



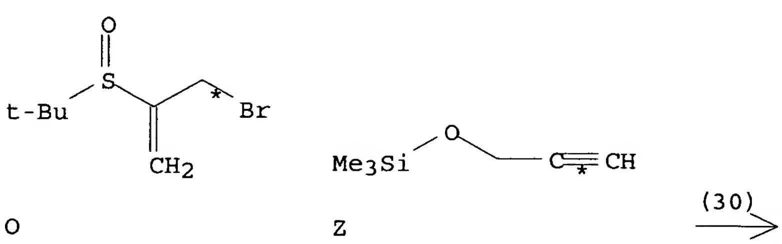
BF Z



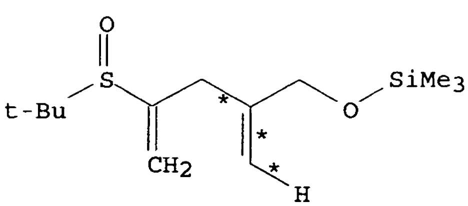
BI
YIELD 48%

RX(29) RCT BF 97147-24-5, Z 5582-62-7
RGT W 7440-66-6 Zn, X 106-93-4 BrCH2CH2Br
PRO BI 107345-32-4
SOL 109-99-9 THF

RX(30) OF 130 ...O + Z ===> BJ...



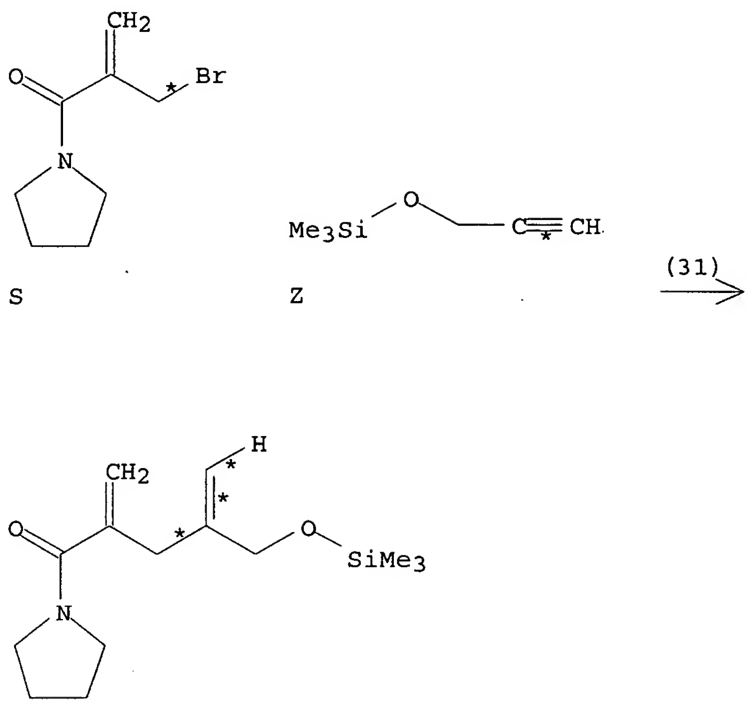
O Z



BJ

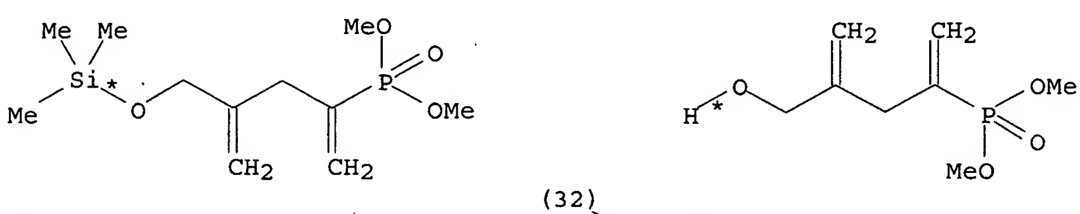
RX(30) RCT O 107345-23-3, Z 5582-62-7
RGT W 7440-66-6 Zn, X 106-93-4 BrCH2CH2Br
PRO BJ 107345-33-5
SOL 109-99-9 THF

RX(31) OF 130 ...S + Z ===> BK...



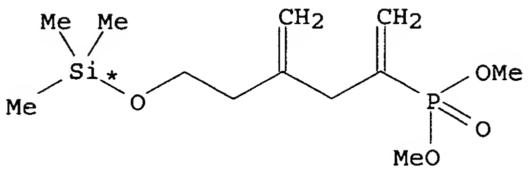
RX(31) RCT S 107345-24-4, Z 5582-62-7
RGT W 7440-66-6 Zn, X 106-93-4 BrCH2CH2Br
PRO BK 107345-34-6
SOL 109-99-9 THF

RX(32) OF 130 ...AY ===> BL...



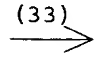
RX(32) RCT AY 107345-27-7
RGT BM 7647-01-0 HCl
PRO BL 91476-21-0
SOL 7732-18-5 Water

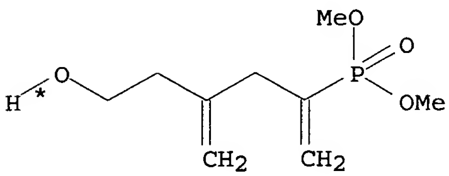
RX(33) OF 130 ...AZ ===> BO...



AZ

(33)

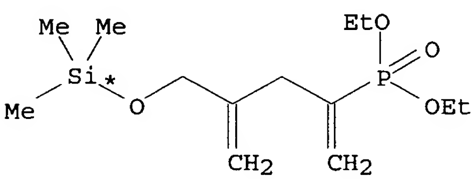




BO

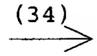
RX(33) RCT AZ 107345-28-8
RGT BM 7647-01-0 HCl
PRO BO 91476-22-1
SOL 7732-18-5 Water

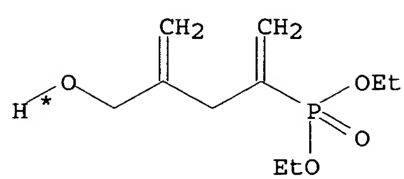
RX(34) OF 130 ...BA ===> BP...



BA

(34)

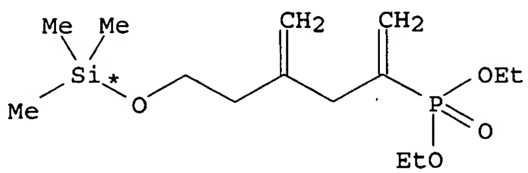




BP

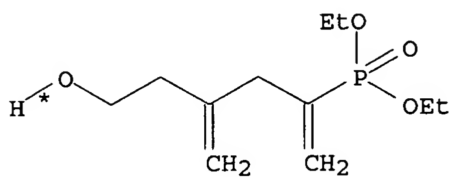
RX(34) RCT BA 107345-29-9
RGT BM 7647-01-0 HCl
PRO BP 91476-23-2
SOL 7732-18-5 Water

RX(35) OF 130 ...BB ===> BQ...



BB

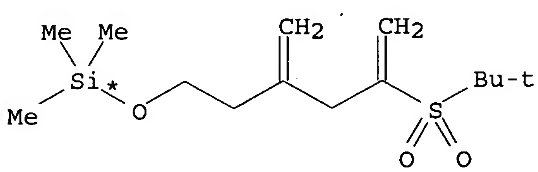
(35) $\longrightarrow$



BQ

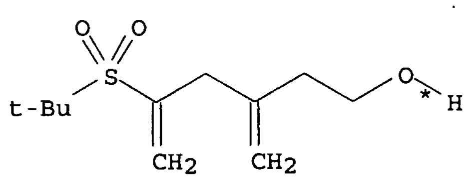
RX(35)   RCT BB 107345-30-2
           RGT BM 7647-01-0 HCl
           PRO BQ 91476-24-3
           SOL 7732-18-5 Water

RX(36) OF 130   ...BH ===> BR



BH

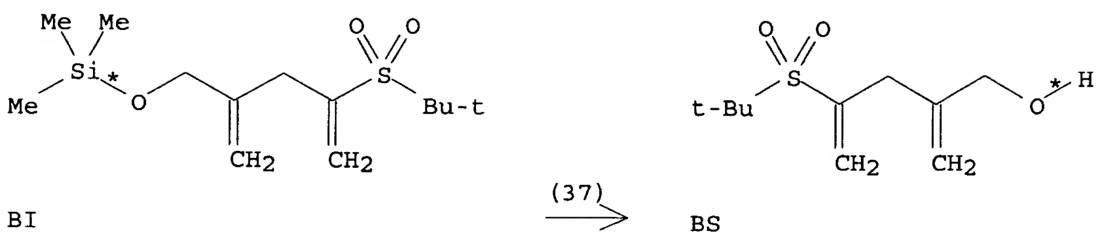
(36) $\longrightarrow$



BR

RX(36)   RCT BH 107345-31-3
           RGT BM 7647-01-0 HCl
           PRO BR 97779-26-5
           SOL 7732-18-5 Water

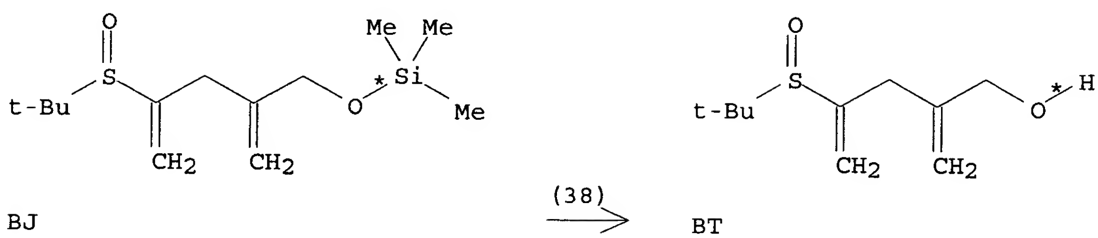
RX(37) OF 130   ...BI ===> BS



BI (37) BS

RX(37) RCT BI 107345-32-4
RGT BM 7647-01-0 HCl
PRO BS 97779-25-4
SOL 7732-18-5 Water

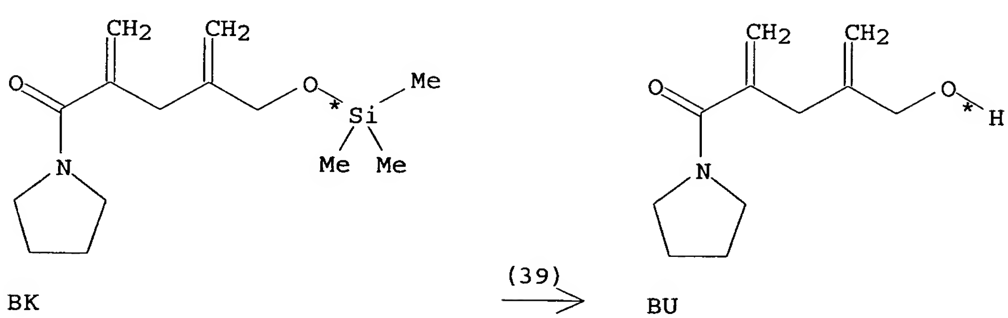
RX(38) OF 130 ...BJ ===> BT



BJ (38) BT

RX(38) RCT BJ 107345-33-5
RGT BM 7647-01-0 HCl
PRO BT 107345-35-7
SOL 7732-18-5 Water

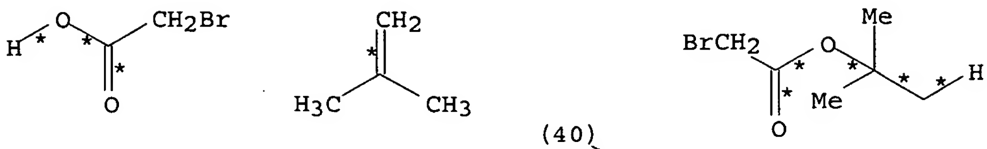
RX(39) OF 130 ...BK ===> BU



BK (39) BU

RX(39) RCT BK 107345-34-6
RGT BM 7647-01-0 HCl
PRO BU 107345-36-8
SOL 7732-18-5 Water

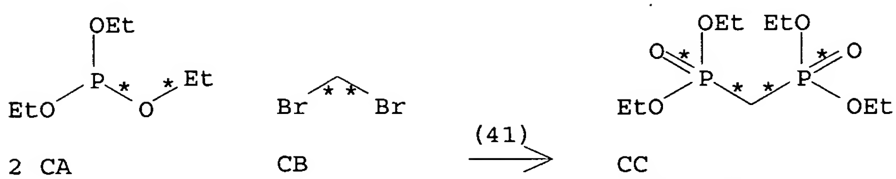
RX(40) OF 130 BV + BW ===> BX



BV BW BX
YIELD 86%

RX(40) RCT BV 79-08-3, BW 115-11-7
RGT BY 9037-24-5 Amberlyst 15
PRO BX 5292-43-3
SOL 67-66-3 CHCl3

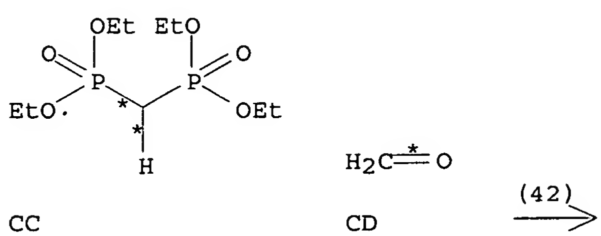
RX(41) OF 130 2 CA + CB ===> CC...



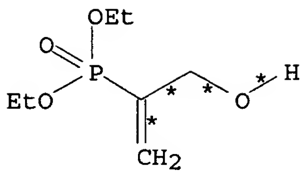
2 CA CB CC
YIELD 66%

RX(41) RCT CA 122-52-1, CB 74-95-3
PRO CC 1660-94-2

RX(42) OF 130 ...CC + CD ===> F...



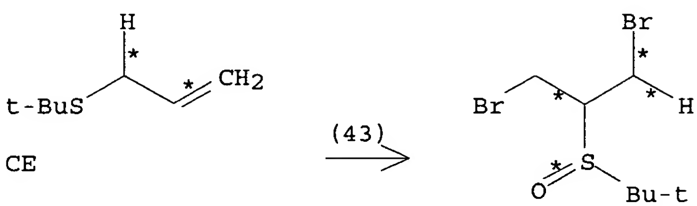
CC CD



F
YIELD 60%

RX(42) RCT CC 1660-94-2, CD 50-00-0
PRO F 93032-43-0
SOL 7732-18-5 Water

RX(43) OF 130 CE ===> N...



N
YIELD 56%

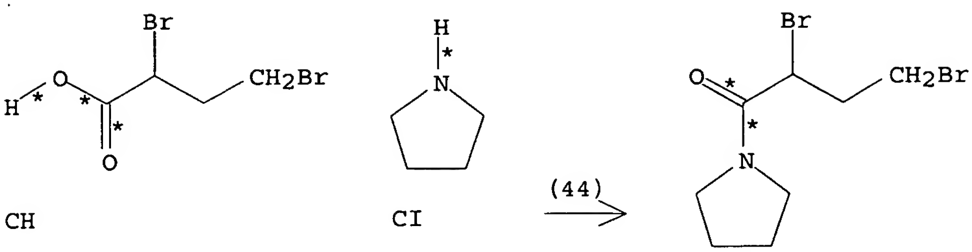
RX(43) RCT CE 37850-75-2

STAGE(1)
RGT CF 7726-95-6 Br2
SOL 56-23-5 CCl4

STAGE(2)
RGT CG 937-14-4 MCPBA
SOL 75-09-2 CH2Cl2

PRO N 107345-37-9

RX(44) OF 130 CH + CI ===> R...



CH CI R

YIELD 26%

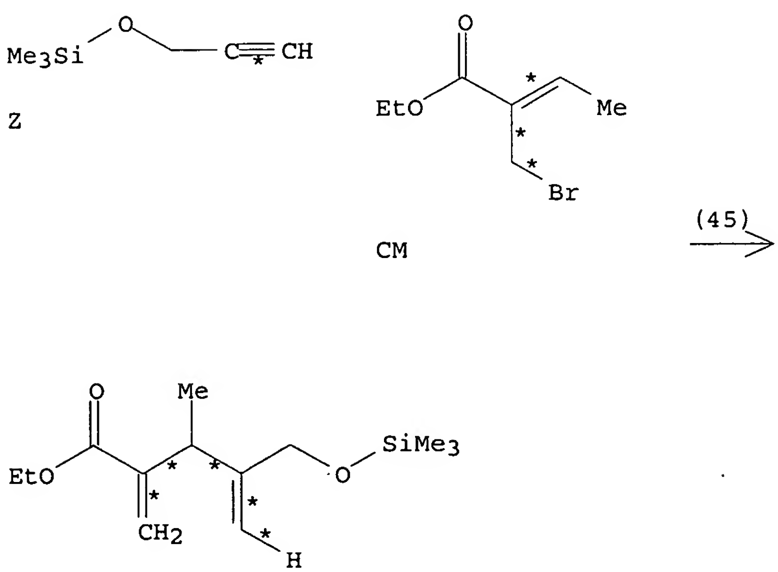
RX(44) RCT CH 63164-16-9

STAGE(1)
RGT CJ 7719-09-7 SOCl2, CK 68-12-2 DMF
SOL 75-09-2 CH2Cl2

STAGE(2)
RCT CI 123-75-1
RGT CL 110-86-1 Pyridine
SOL 60-29-7 Et2O

PRO R 107345-38-0

RX(45) OF 130 Z + CM ===> CN



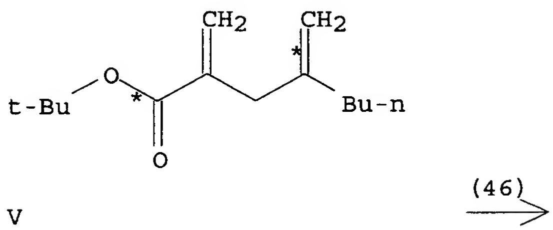
Z CM

CN
YIELD 71%

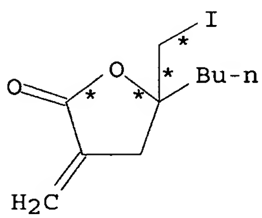
RX(45) RCT Z 5582-62-7, CM 62097-05-6
RGT W 7440-66-6 Zn, X 106-93-4 BrCH2CH2Br

PRO CN 107345-40-4
SOL 109-99-9 THF

RX(46) OF 130 ...V ===> CO



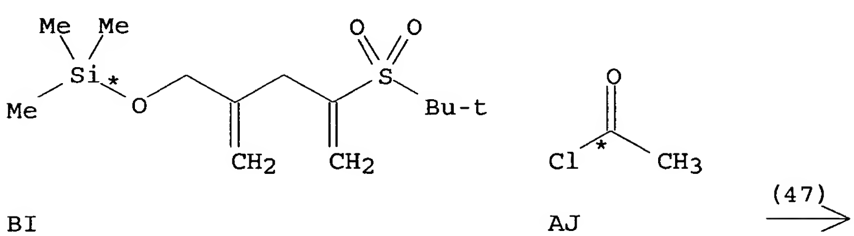
V



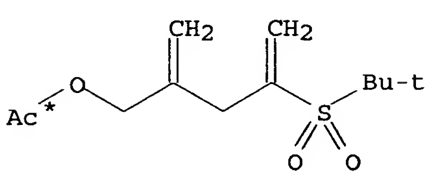
CO
YIELD 90%

RX(46) RCT V 91476-11-8
RGT CP 7553-56-2 I2, CQ 584-08-7 K2CO3
PRO CO 91476-25-4

RX(47) OF 130 ...BI + AJ ===> CR...



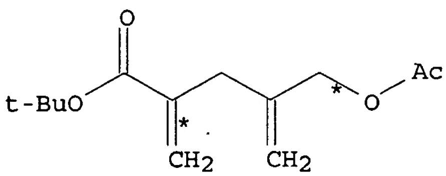
BI AJ



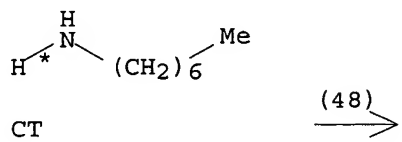
CR
YIELD 89%

RX(47) RCT BI 107345-32-4, AJ 75-36-5
RGT AK 64-19-7 AcOH, CS 1122-58-3 4-DMAP
PRO CR 107345-42-6
SOL 60-29-7 Et2O, 64-19-7 AcOH

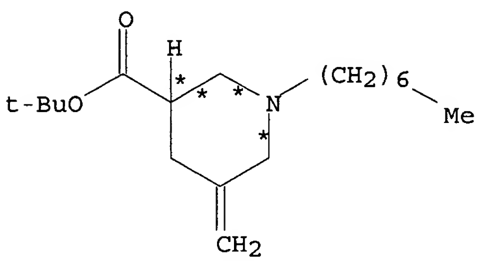
RX(48) OF 130 ...AI + CT ===> CU



AI



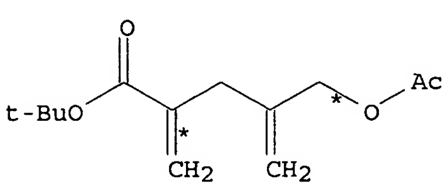
CT



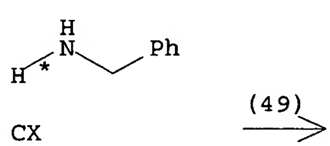
CU
YIELD 82%

RX(48) RCT AI 91476-26-5, CT 111-68-2
RGT CV 121-44-8 Et3N, CW 14221-01-3 Pd(PPh3)4
PRO CU 91476-28-7
SOL 109-99-9 THF

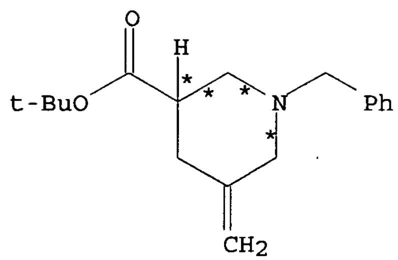
RX(49) OF 130 ...AI + CX ===> CY



AI



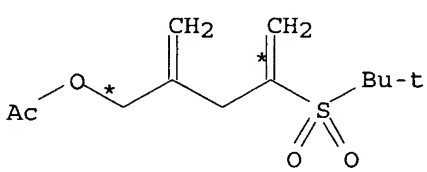
CX



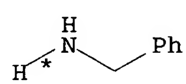
CY
YIELD 76%

RX(49) RCT AI 91476-26-5, CX 100-46-9
RGT CV 121-44-8 Et3N, CW 14221-01-3 Pd(PPh3)4
PRO CY 91476-29-8
SOL 109-99-9 THF

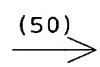
RX(50) OF 130 ...CR + CX ===> CZ

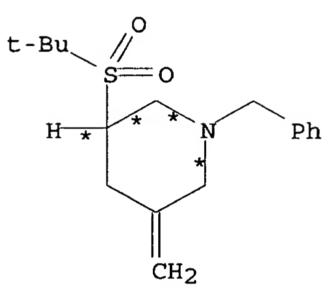


CR



CX

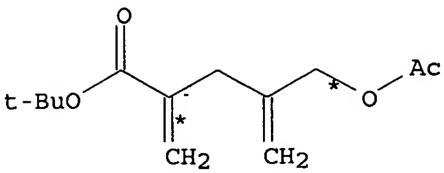




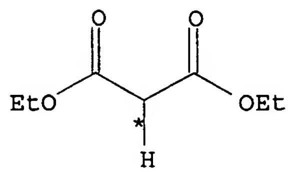
CZ
YIELD 90%

RX(50) RCT CR 107345-42-6, CX 100-46-9
RGT CW 14221-01-3 Pd(PPh3)4, DA 7646-69-7 NaH
PRO CZ 107345-43-7
SOL 109-99-9 THF

RX(51) OF 130 ...**AI** + **DB** ===> **DC**

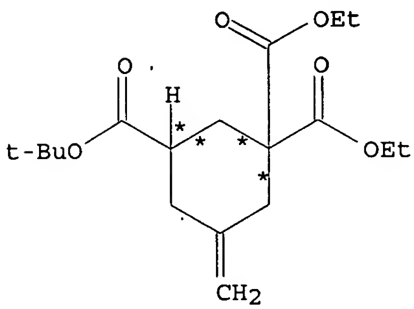


AI



DB

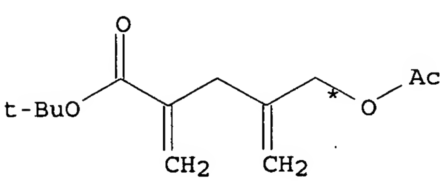
(51) →



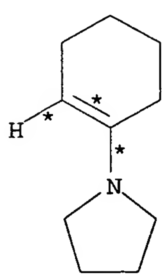
DC
YIELD 70%

RX(51) RCT AI **91476-26-5**, DB **105-53-3**
RGT CW **14221-01-3** Pd(PPh3)4, DA 7646-69-7 NaH
PRO DC **91476-27-6**
SOL 109-99-9 THF

RX(52) OF 130 ...AI + DD ===> DE

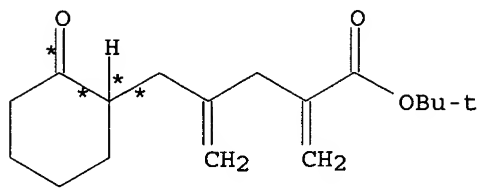


AI



DD

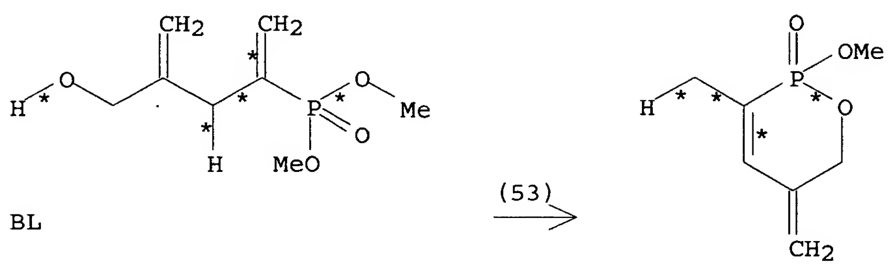
(52) →



DE
YIELD 50%

RX(52) RCT AI 91476-26-5, DD 1125-99-1
RGT CV 121-44-8 Et3N, CW 14221-01-3 Pd(PPh3)4
PRO DE 91476-30-1
SOL 75-05-8 MeCN

RX(53) OF 130 ...BL ===> DG

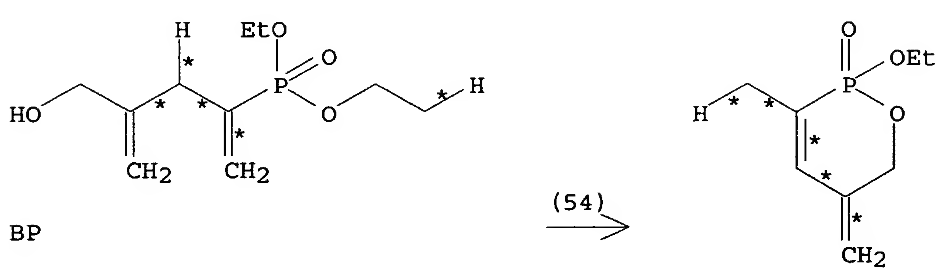


BL

DG
YIELD 95%

RX(53) RCT BL 91476-21-0
RGT DA 7646-69-7 NaH
PRO DG 91476-31-2
SOL 109-99-9 THF

RX(54) OF 130 ...BP ===> DH

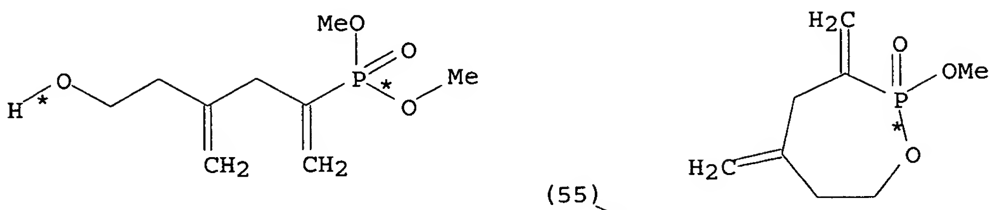


BP

DH
YIELD 95%

```
RX(54)      RCT   BP 91476-23-2
            RGT   DA 7646-69-7 NaH
            PRO   DH 91476-32-3
            SOL   109-99-9 THF
```

RX(55) OF 130 ...BO ===> DI

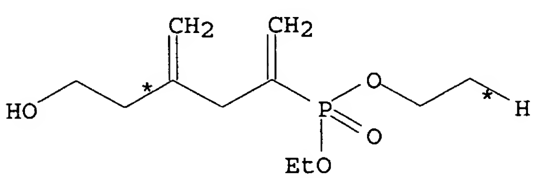


BO

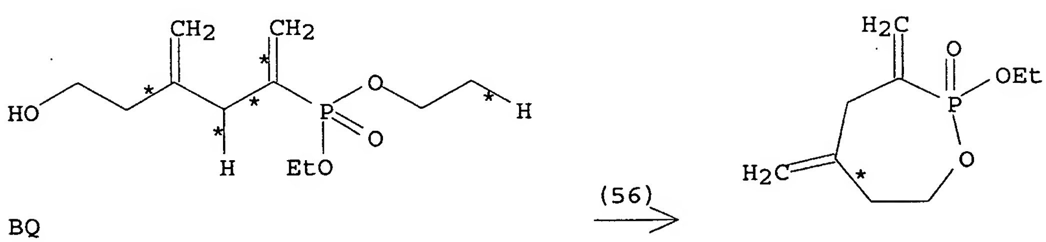
DI
YIELD 78%

```
RX(55)      RCT   BO 91476-22-1
            RGT   DA 7646-69-7 NaH
            PRO   DI 91476-33-4
            SOL   109-99-9 THF
```

RX(56) OF 130 ...2 BQ ===> DJ + DK

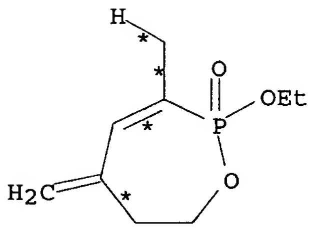


BQ



BQ

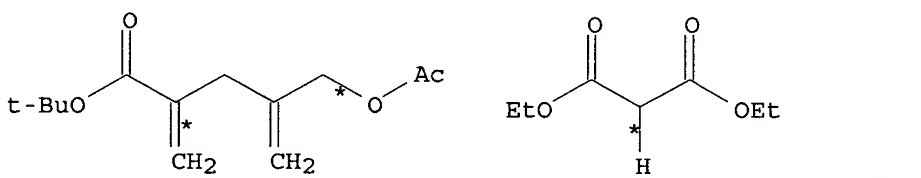
DJ
YIELD 64%(85)



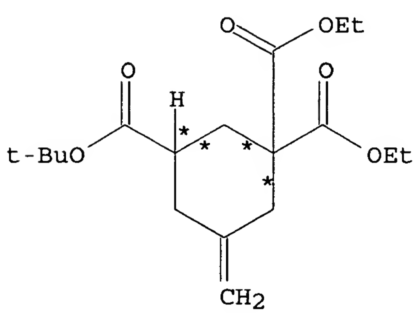
DK
YIELD 64%(15)

RX(56) RCT BQ 91476-24-3
RGT DA 7646-69-7 NaH
PRO DJ 107345-44-8, DK 107345-45-9
SOL 109-99-9 THF

RX(51) OF 130 ...**AI** + **DB** ===> **DC**



AI DB

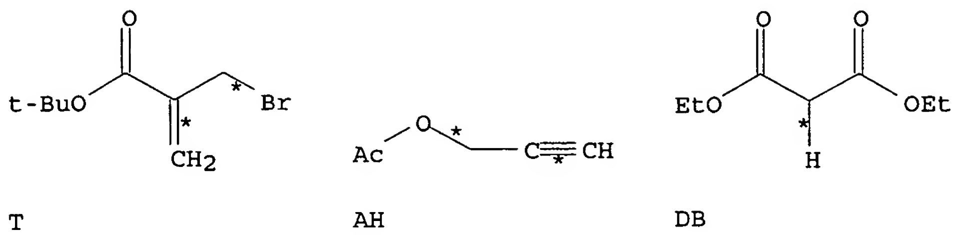


DC
YIELD 70%

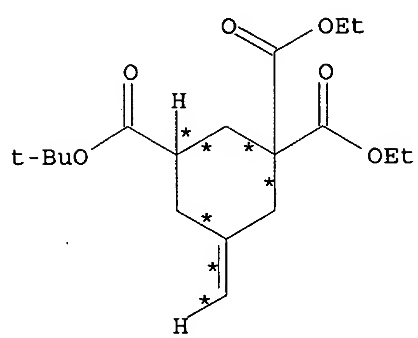
RX(51) RCT AI **91476-26-5**, DB **105-53-3**
RGT CW **14221-01-3** Pd(PPh3)4, DA 7646-69-7 NaH
PRO DC **91476-27-6**
SOL 109-99-9 THF

RX(71) OF 130 COMPOSED OF RX(11), RX(51)

RX(71) **T** + AH + **DB** ===> **DC**



2
STEPS

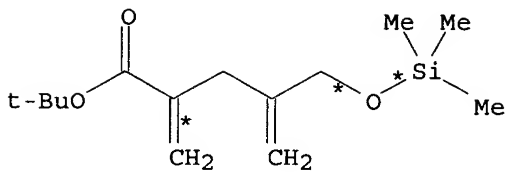


DC
YIELD 70%

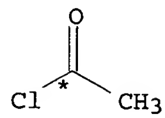
RX(11) RCT T **53913-96-5**, AH 627-09-8
RGT W 7440-66-6 Zn, X 106-93-4 BrCH2CH2Br
PRO AI 91476-26-5
SOL 109-99-9 THF

RX(51) RCT AI 91476-26-5, DB **105-53-3**
RGT CW **14221-01-3** Pd(PPh3)4, DA 7646-69-7 NaH
PRO DC **91476-27-6**
SOL 109-99-9 THF

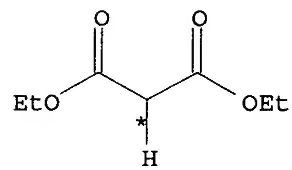
RX(75) OF 130 COMPOSED OF RX(12), RX(51)
RX(75) **AA** + AJ + **DB** ===> **DC**



AA

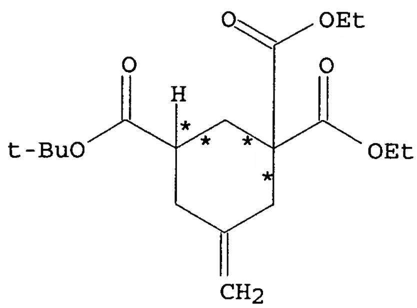


AJ



DB

2
STEPS
→

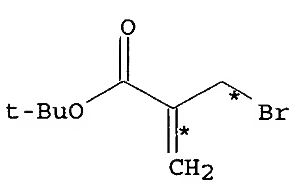


DC
YIELD 70%

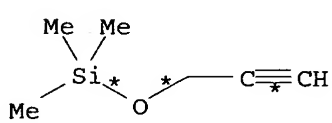
RX(12) RCT AA **91476-12-9**, AJ 75-36-5
RGT AK 64-19-7 AcOH
PRO AI 91476-26-5
SOL 60-29-7 Et2O, 64-19-7 AcOH

RX(51) RCT AI 91476-26-5, DB **105-53-3**
RGT CW **14221-01-3** Pd(PPh3)4, DA 7646-69-7 NaH
PRO DC **91476-27-6**
SOL 109-99-9 THF

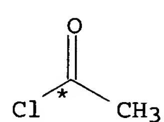
RX(107) OF 130 COMPOSED OF RX(7), RX(12), RX(51)
RX(107) **T** + Z + AJ + **DB** ===> **DC**



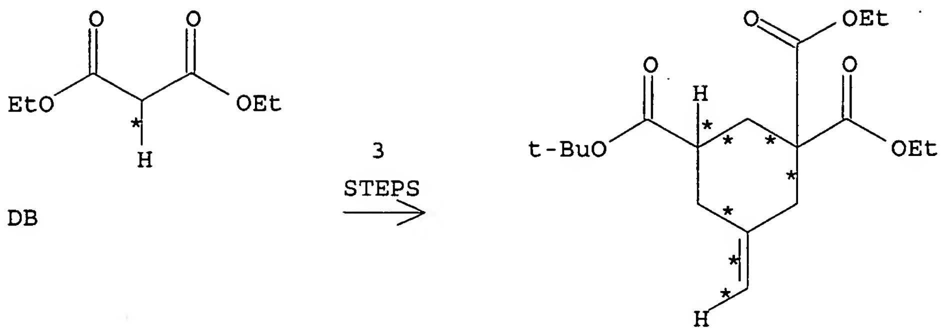
T



Z



AJ



DB

3
STEPS

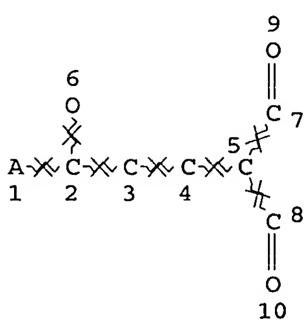
DC
YIELD 70%

```
RX(7)       RCT  T 53913-96-5, Z 5582-62-7
            RGT  W 7440-66-6 Zn, X 106-93-4 BrCH2CH2Br
            PRO  AA 91476-12-9
            SOL  109-99-9 THF

RX(12)      RCT  AA 91476-12-9, AJ 75-36-5
            RGT  AK 64-19-7 AcOH
            PRO  AI 91476-26-5
            SOL  60-29-7 Et2O, 64-19-7 AcOH

RX(51)      RCT  AI 91476-26-5, DB 105-53-3
            RGT  CW 14221-01-3 Pd(PPh3)4, DA 7646-69-7 NaH
            PRO  DC 91476-27-6
            SOL  109-99-9 THF

=> => d que stat l93
L21              SCR 1918 OR 2043 OR 1840 OR 1949 OR 2010
L25              STR
```



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NODE ATTRIBUTES:
CONNECT IS X2   RC AT   6
CONNECT IS E1   RC AT   9
CONNECT IS E1   RC AT  10
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
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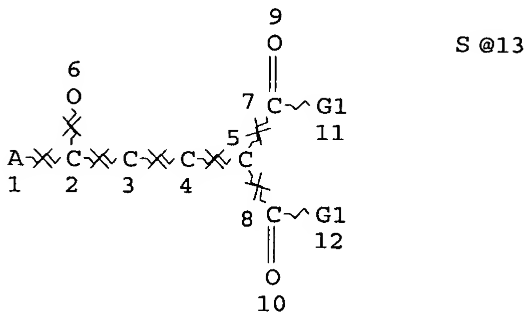
NUMBER OF NODES IS 10

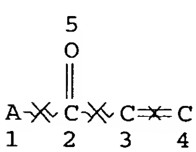
STEREO ATTRIBUTES: NONE
L27 12118 SEA FILE=REGISTRY SSS FUL L25 NOT L21
L30 STR



VAR G1=O/N/P/13
NODE ATTRIBUTES:
CONNECT IS X2 RC AT 6
CONNECT IS E1 RC AT 9
CONNECT IS E1 RC AT 10
CONNECT IS X2 RC AT 13
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 13

STEREO ATTRIBUTES: NONE
L32 2503 SEA FILE=REGISTRY SUB=L27 SSS FUL L30
L37 STR



NODE ATTRIBUTES:
CONNECT IS E1 RC AT 5
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 5

STEREO ATTRIBUTES: NONE
L40 SCR 1918 OR 2043 OR 1839 OR 1944 OR 2005
L42 6815 SEA FILE=REGISTRY SSS FUL L37 NOT L40
L50 1507 SEA FILE=HCAPLUS ABB=ON PLU=ON L32/P
L51 31232 SEA FILE=HCAPLUS ABB=ON PLU=ON L42/RACT
L52 266 SEA FILE=HCAPLUS ABB=ON PLU=ON L50 AND L51
L53 QUE ABB=ON PLU=ON "ASYMMETRIC SYNTHESIS AND INDUCTIO
N"+PFT,OLD,NT/CT
L54 QUE ABB=ON PLU=ON "MICHAEL REACTION"+PFT,OLD,NT/CT
L55 QUE ABB=ON PLU=ON "MICHAEL REACTION CATALYSTS"+PFT,O

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                LD,NT/CT
L56          30 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L53 AND L52
L57          21 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L56 AND (L54 OR L55)
L60       31232 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L42/RACT
L61        1337 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L60 AND L53
L62         176 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L61 AND (L54 OR L55)
L63          92 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L62 AND L55
L64      744935 SEA FILE=REGISTRY ABB=ON  PLU=ON  ((FE OR CO OR NI OR
                RU OR RH OR PD OR OS OR IR OR PT)(L)N)/ELS
L66      316118 SEA FILE=REGISTRY ABB=ON  PLU=ON  L64 AND 1-2/N
L67      262888 SEA FILE=REGISTRY ABB=ON  PLU=ON  L66 AND 1/M
L68       22790 SEA FILE=REGISTRY ABB=ON  PLU=ON  L67 AND 1/RU
L69       80253 SEA FILE=REGISTRY ABB=ON  PLU=ON  L67 AND (1/OS OR
                1/IR OR 1/PT OR 1/PD)
L70      159878 SEA FILE=REGISTRY ABB=ON  PLU=ON  L67 NOT (L68 OR L69)

L71       76518 SEA FILE=REGISTRY ABB=ON  PLU=ON  L70 AND 1/FE
L72       83360 SEA FILE=REGISTRY ABB=ON  PLU=ON  L67 NOT (L68 OR L69
                OR L71)
L73             QUE  ABB=ON  PLU=ON  L68
L74             QUE  ABB=ON  PLU=ON  L69
L75             QUE  ABB=ON  PLU=ON  L71
L76             QUE  ABB=ON  PLU=ON  L72
L77             QUE  ABB=ON  PLU=ON  L73 OR L74 OR L75 OR L76
L78          10 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L63 AND L77
L80        9613 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L27
L81       50879 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L42
L82          31 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L80 AND L81 AND L77
L83           7 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L82 AND L53
L84        1971 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L32
L85         315 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L84 AND L42
L86          14 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L85 AND L77
L87          39 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L57 OR L78 OR L83 OR
                L86
L89          62 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L87 OR L56 OR L82
L90          48 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L89 AND (L53 OR L54
                OR L55)
L92             QUE  ABB=ON  PLU=ON  PY<2005 OR PRY<2005 OR AY<2005 OR
                MY<2005 OR REVIEW/DT
L93          34 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L90 AND L92


=> d l93 1-34 ibib abs ed hitstr hitind

L93  ANSWER 1 OF 34  HCAPLUS  COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER:         2004:792305  HCAPLUS
DOCUMENT NUMBER:          141:424327
TITLE:                    Enantioselective total synthesis of
                          (-)-strychnine: development of a highly
                          practical catalytic asymmetric carbon-carbon
                          bond formation and domino cyclization
AUTHOR(S):                Ohshima, Takashi; Xu, Youjun; Takita, Ryo;
                          Shibasaki, Masakatsu
CORPORATE SOURCE:         Graduate School of Pharmaceutical Sciences,
                          The University of Tokyo, Hongo, Bunkyo-ku,
                          Tokyo, 113-0033, Japan
SOURCE:                   Tetrahedron (2004), 60(43),
                          9569-9588
                          CODEN: TETRAB; ISSN: 0040-4020
PUBLISHER:                Elsevier B.V.
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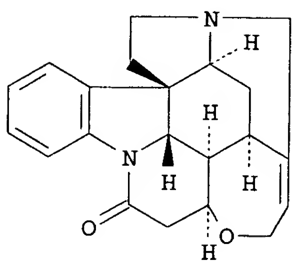
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 141:424327
GI



I

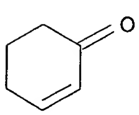
AB An enantioselective total synthesis of (-)-strychnine (I) was accomplished through the use of the highly practical catalytic asym. Michael reaction (0.1 mol% of (R)-ALB, greater than kilogram scale, without chromatog., 91% yield and >99% ee), and a domino cyclization that simultaneously constructed the B- and D- rings of strychnine (>77% yield). Newly-developed reaction conditions for thionium ion cyclization, NaBH3CN reduction of the imine moiety in the presence of a Lewis acid to prevent the ring-opening reaction, and chemoselective reduction of the thioether (desulfurization) in the presence of exocyclic olefin were pivotal to complete the synthesis. The described chemical paves the way for the synthesis of more advanced Strychnos alkaloids.

ED Entered STN: 29 Sep 2004

IT **930-68-7**, 2-Cyclohexenone
RL: RCT (Reactant); **RACT (Reactant or reagent)**
(enantioselective total synthesis of (-)-strychnine via catalytic asym. Michael reaction and domino cyclization)

RN 930-68-7 HCAPLUS

CN 2-Cyclohexen-1-one (6CI, 8CI, 9CI) (CA INDEX NAME)

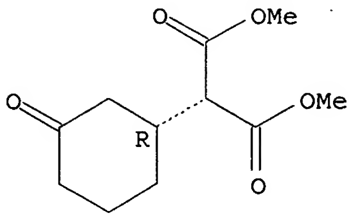


IT **164931-77-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(enantioselective total synthesis of (-)-strychnine via catalytic asym. Michael reaction and domino cyclization)

RN 164931-77-5 HCAPLUS

CN Propanedioic acid, [(1R)-3-oxocyclohexyl]-, dimethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



CC 31-5 (Alkaloids)
IT **Asymmetric synthesis and induction**
Cyclization
(enantioselective total synthesis of (-)-strychnine via catalytic asym. Michael reaction and domino cyclization)
IT **Michael reaction**
(stereoselective; enantioselective total synthesis of (-)-strychnine via catalytic asym. Michael reaction and domino cyclization)
IT 108-59-8, Dimethyl malonate 126-39-6 609-73-4, 1-Iodo-2-nitrobenzene 661-69-8, Hexamethyldistannane **930-68-7**, 2-Cyclohexenone 22483-09-6 122807-21-0 191731-32-5
RL: RCT (Reactant); **RACT (Reactant or reagent)**
(enantioselective total synthesis of (-)-strychnine via catalytic asym. Michael reaction and domino cyclization)
IT 509-40-0P, Diaboline 71366-23-9P 76074-18-5P **164931-77-5P** 482351-05-3P 482351-06-4P 482351-07-5P 482351-08-6P 482351-09-7P 482351-10-0P 482351-11-1P 482351-12-2P 482351-13-3P 482351-14-4P 482351-15-5P 482351-16-6P 482351-18-8P 482351-19-9P 482351-20-2P 482351-22-4P 482351-24-6P 482351-25-7P 482351-26-8P 482351-27-9P 482351-28-0P 482351-29-1P 482351-31-5P 793723-96-3P 793723-97-4P 793723-98-5P 793724-03-5P 793724-04-6P 793724-09-1P 793724-10-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(enantioselective total synthesis of (-)-strychnine via catalytic asym. Michael reaction and domino cyclization)
REFERENCE COUNT: 103 THERE ARE 103 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L93 ANSWER 2 OF 34 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2004:584477 HCAPLUS
DOCUMENT NUMBER: 141:140101
TITLE: Process and catalysts for producing optically active cycloalkylmalonates
INVENTOR(S): Watanabe, Masahito; Murata, Kunihiko; Ikariya, Takao
PATENT ASSIGNEE(S): Kanto Kagaku Kabushiki Kaisha, Japan
SOURCE: Eur. Pat. Appl., 29 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE

EP 1439159	A1	20040721	EP 2004-296	2004 0109 <--

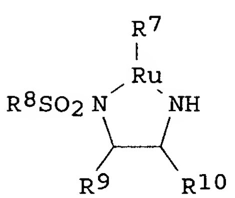
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK

JP 2004269481	A2	20040930	JP 2003-71368	2003 0317 <--
US 2004176616	A1	20040909	US 2003-749806	2003 1231 <--

PRIORITY APPLN. INFO.: JP 2003-9786 A 2003 0117 <--
JP 2003-71368 A 2003 0317 <--

OTHER SOURCE(S): MARPAT 141:140101

GI



I

AB Optically active malonate derivs. R1COCR2R3CR4(COXR5)COYR6 [R1 = (un)substituted aromatic, aliphatic, alicyclic, heterocyclic, H, alkoxy, amino; R2-R4 = H, (un)substituted aryl, aliphatic, alicyclic, heterocyclic; R1R2, R1R3, R2R3, R4R5, R5R6, R4R6 = atoms required to form a ring; R5, R6 = H, (un)substituted aryl, aliphatic, alicyclic, alkoxy; X, Y = bond; XR5, YR6 = (un)substituted OH, NH2] were prepared by treating R1COCH:CR2R3 with R4CH(COXR5)COYR6 in presence of an asym. metal catalyst, preferably a Ru catalyst I [R7-R10 = (un)substituted Ph]. Thus, [RuCl2(C6Me6)]2 was treated with (S,S)-TsDPEN to give Ru[(S,S)-TsDPEN](C6Me6) which was used in the Michael reaction of 2-cyclohexenone with CH2(CO2Me)2 to give (R)-3-[bis(methoxycarbonyl)methyl]cyclohexanone in 96% ee.

ED Entered STN: 22 Jul 2004

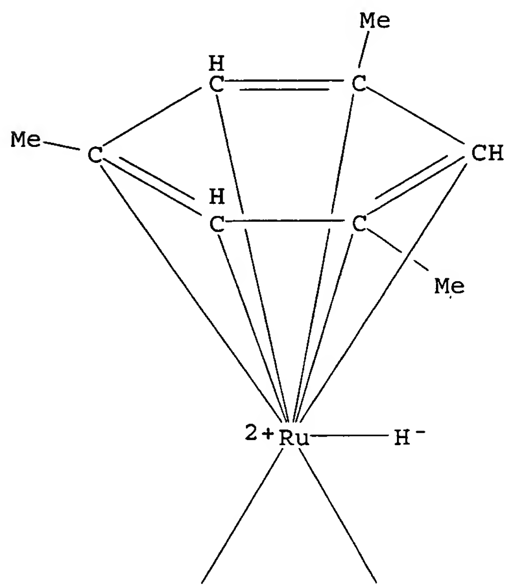
IT **725737-68-8P**

RL: CAT (Catalyst use); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

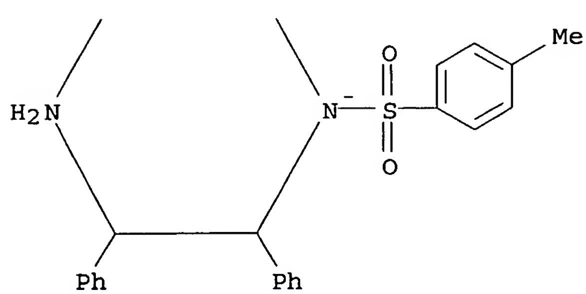
(process and catalysts for producing optically active cycloalkylmalonates)

RN 725737-68-8 HCAPLUS
CN Ruthenium, [N-[(1R,2R)-2-(amino-κN)-1,2-diphenylethyl]-4-methylbenzenesulfonamidato-κN]hydro[(1,2,3,4,5,6-η)-1,3,5-trimethylbenzene]- (9CI) (CA INDEX NAME)

PAGE 1-A

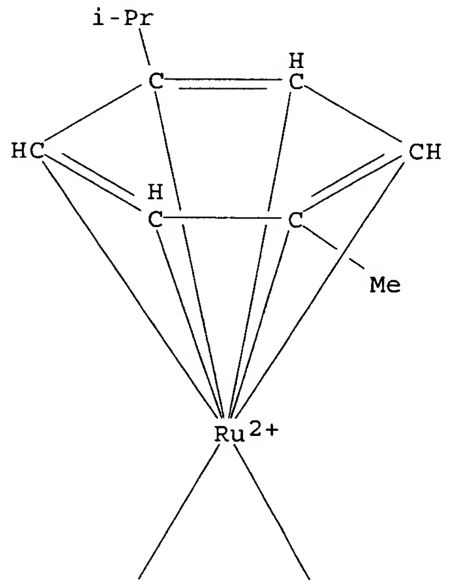


PAGE 2-A



IT **188444-42-0P 725737-67-7P 725737-69-9P 725737-70-2P 725737-71-3P**
RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(process and catalysts for producing optically active cycloalkylmalonates)
RN 188444-42-0 HCAPLUS
CN Ruthenium, [N-[(1S,2S)-2-(amino-κN)-1,2-diphenylethyl]-4-methylbenzenesulfonamidato(2-)-κN][(1,2,3,4,5,6-η)-1-methyl-4-(1-methylethyl)benzene]- (9CI) (CA INDEX NAME)

PAGE 1-A



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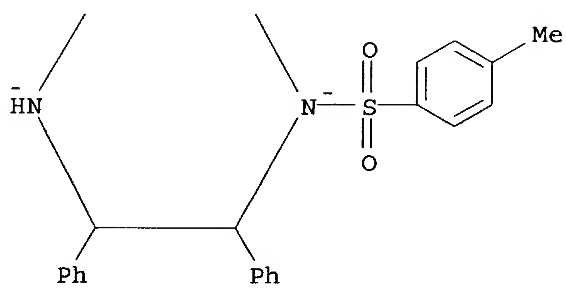
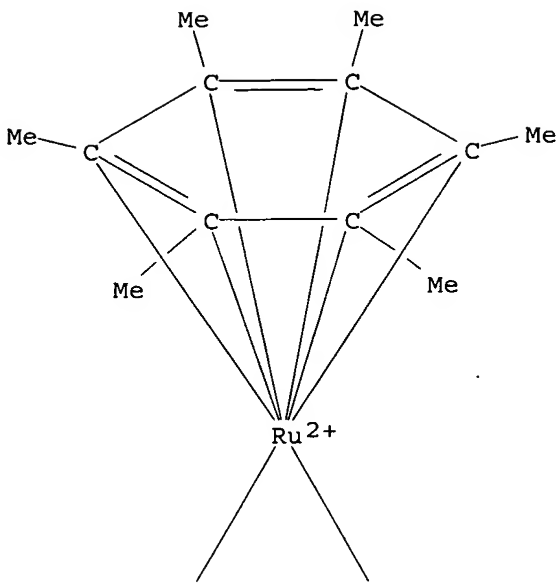


RN 725737-67-7 HCAPLUS
CN Ruthenium, [N-[(1S,2S)-2-(amino-κN)-1,2-diphenylethyl]-4-methylbenzenesulfonamidato(2-)-κN][(1,2,3,4,5,6-η)-hexamethylbenzene]- (9CI) (CA INDEX NAME)

PAGE 1-A



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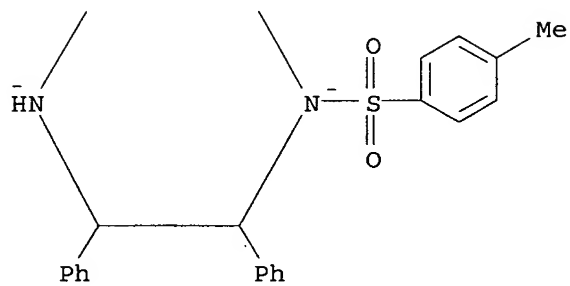
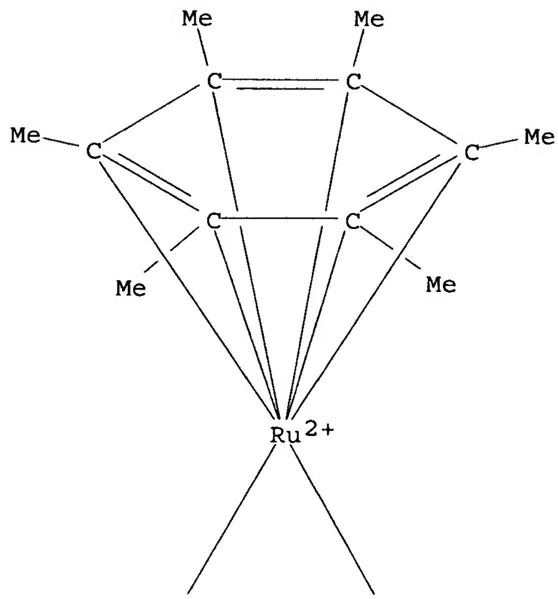


RN 725737-69-9 HCAPLUS
CN Ruthenium, [N-[(1S,2S)-2-(amino-κN)-1,2-diphenylethyl]methanesulfonamidato(2-)-κN][(1,2,3,4,5,6-η)-hexamethylbenzene]- (9CI) (CA INDEX NAME)

PAGE 1-A



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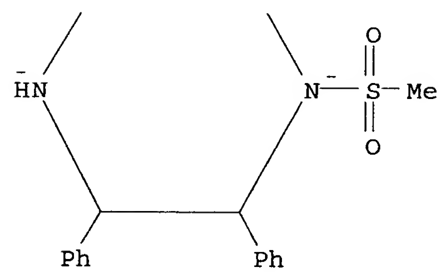
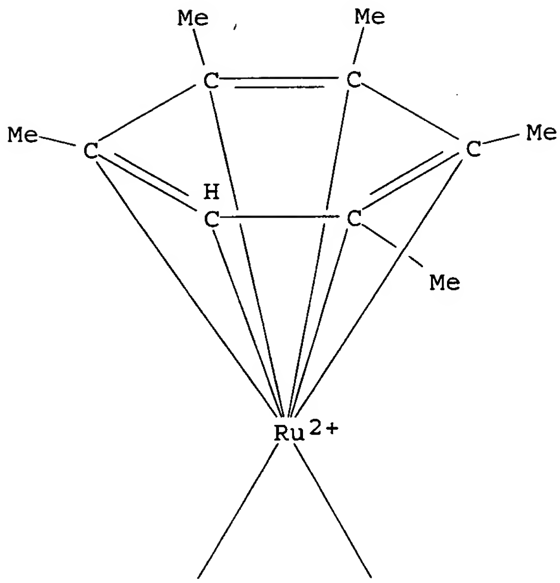


RN 725737-70-2 HCAPLUS
CN Ruthenium, [N-[(1S,2S)-2-(amino-κN)-1,2-diphenylethyl]-4-methylbenzenesulfonamidato(2-)-κN][(1,2,3,4,5,6-η)-pentamethylbenzene]- (9CI) (CA INDEX NAME)

PAGE 1-A



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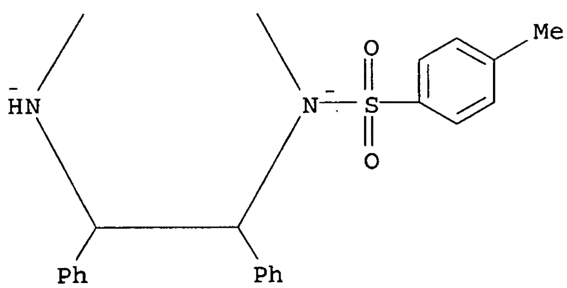
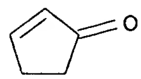
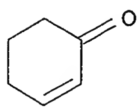


RN 725737-71-3 HCAPLUS
CN Ruthenium, [N-[(1R,2R)-2-(amino-κN)-1,2-diphenylethyl]-4-methylbenzenesulfonamidato(2-)-κN](dimethyl propanedioate-κO1',κO3')[(1,2,3,4,5,6-η)-1,3,5-trimethylbenzene]- (9CI) (CA INDEX NAME)

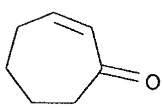
*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
IT **930-30-3**, 2-Cyclopentenone **930-68-7**, 2-Cyclohexenone **1121-66-0**, 2-Cycloheptenone **22748-16-9**, 4,4-Dimethyl-2-cyclopentenone
RL: RCT (Reactant); **RACT (Reactant or reagent)**
(process and catalysts for producing optically active cycloalkylmalonates)
RN 930-30-3 HCAPLUS
CN 2-Cyclopenten-1-one (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



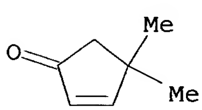
RN 930-68-7 HCAPLUS
CN 2-Cyclohexen-1-one (6CI, 8CI, 9CI) (CA INDEX NAME)



RN 1121-66-0 HCAPLUS
CN 2-Cyclohepten-1-one (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

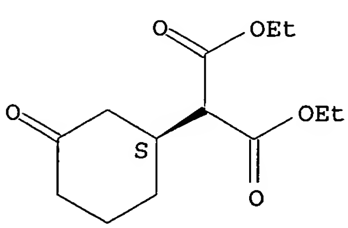


RN 22748-16-9 HCAPLUS
CN 2-Cyclopenten-1-one, 4,4-dimethyl- (7CI, 8CI, 9CI) (CA INDEX NAME)



IT **151600-50-9P 287493-82-7P 724774-83-8P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(process and catalysts for producing optically active cycloalkylmalonates)
RN 151600-50-9 HCAPLUS
CN Propanedioic acid, [(1S)-3-oxocyclohexyl]-, diethyl ester (9CI) (CA INDEX NAME)

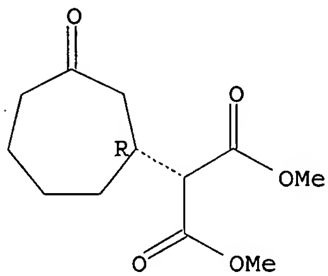
Absolute stereochemistry. Rotation (-).



RN 287493-82-7 HCAPLUS
CN Propanedioic acid, [(1R)-3-oxocycloheptyl]-, dimethyl ester (9CI)

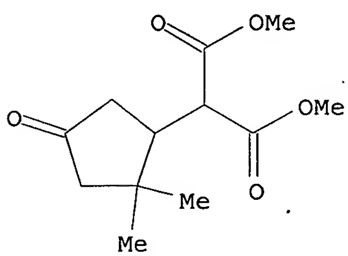
(CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



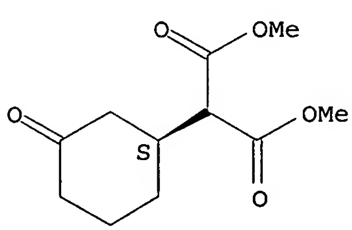
RN 724774-83-8 HCAPLUS
CN Propanedioic acid, (2,2-dimethyl-4-oxocyclopentyl)-, dimethyl ester, (+)- (9CI) (CA INDEX NAME)

Rotation (+).



IT **154194-50-0P 160115-23-1P 164931-77-5P**
164931-78-6P 173837-41-7P 193530-87-9P
194095-90-4P 287493-81-6P 568590-07-8P
569342-29-6P 724774-82-7P, 3-[1,1-Bis(methoxycarbonyl)ethyl]cyclopentanone **724774-84-9P**, 3-[(Acetyl)(methoxycarbonyl)methyl]cyclopentanone
RL: SPN (Synthetic preparation); PREP (Preparation)
(process and catalysts for producing optically active cycloalkylmalonates)
RN 154194-50-0 HCAPLUS
CN Propanedioic acid, [(1S)-3-oxocyclohexyl]-, dimethyl ester (9CI) (CA INDEX NAME)

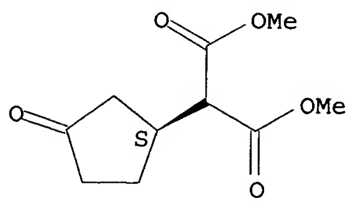
Absolute stereochemistry. Rotation (-).



RN 160115-23-1 HCAPLUS
CN Propanedioic acid, [(1S)-3-oxocyclopentyl]-, dimethyl ester (9CI)

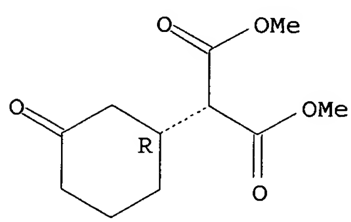
(CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



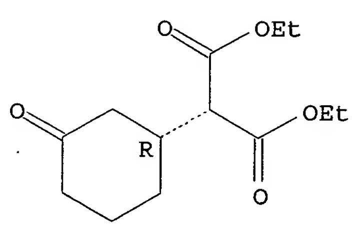
RN 164931-77-5 HCAPLUS
CN Propanedioic acid, [(1R)-3-oxocyclohexyl]-, dimethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



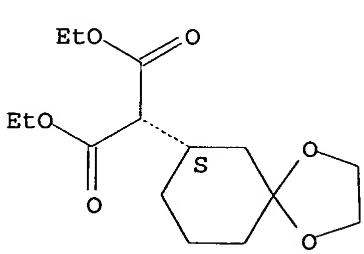
RN 164931-78-6 HCAPLUS
CN Propanedioic acid, [(1R)-3-oxocyclohexyl]-, diethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



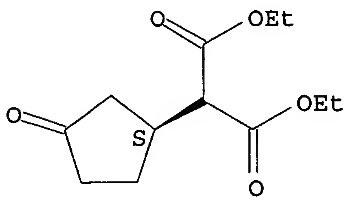
RN 173837-41-7 HCAPLUS
CN Propanedioic acid, (7S)-1,4-dioxaspiro[4.5]dec-7-yl-, diethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



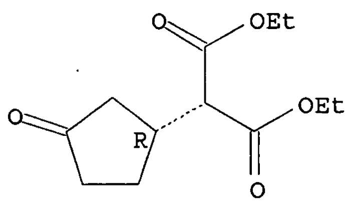
RN 193530-87-9 HCAPLUS
CN Propanedioic acid, [(1S)-3-oxocyclopentyl]-, diethyl ester (9CI)
(CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



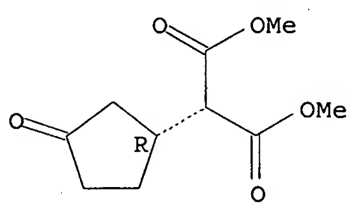
RN 194095-90-4 HCAPLUS
CN Propanedioic acid, [(1R)-3-oxocyclopentyl]-, diethyl ester (9CI)
(CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

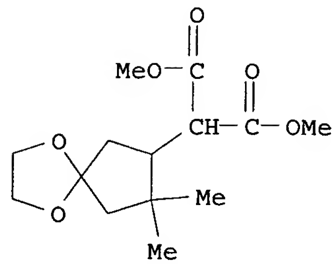


RN 287493-81-6 HCAPLUS
CN Propanedioic acid, [(1R)-3-oxocyclopentyl]-, dimethyl ester (9CI)
(CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

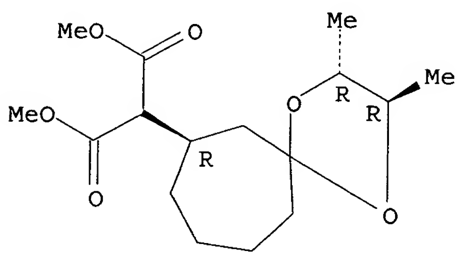


RN 568590-07-8 HCAPLUS
CN Propanedioic acid, (8,8-dimethyl-1,4-dioxaspiro[4.4]non-7-yl)-,
dimethyl ester (9CI) (CA INDEX NAME)

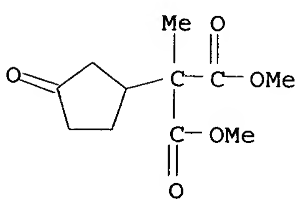


RN 569342-29-6 HCAPLUS
CN Propanedioic acid, [(2R,3R,7R)-2,3-dimethyl-1,4-dioxaspiro[4.6]undec-7-yl]-, dimethyl ester (9CI) (CA INDEX NAME)

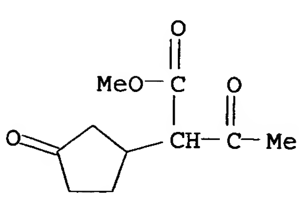
Absolute stereochemistry.



RN 724774-82-7 HCAPLUS
CN Propanedioic acid, methyl(3-oxocyclopentyl)-, dimethyl ester (9CI) (CA INDEX NAME)



RN 724774-84-9 HCAPLUS
CN Cyclopentaneacetic acid, α-acetyl-3-oxo-, methyl ester (9CI) (CA INDEX NAME)



IC ICM C07C045-72
CC 24-5 (Alicyclic Compounds)

IT **Asymmetric synthesis and induction**
(process and catalysts for producing optically active cycloalkylmalonates)
IT **Michael reaction**
Michael reaction catalysts
(stereoselective; process and **catalysts** for producing optically active cycloalkylmalonates)
IT **725737-68-8P**
RL: CAT (Catalyst use); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(process and catalysts for producing optically active cycloalkylmalonates)
IT **188444-42-0P 725737-67-7P 725737-69-9P 725737-70-2P 725737-71-3P**
RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(process and catalysts for producing optically active cycloalkylmalonates)
IT 105-45-3, Methyl acetoacetate 105-53-3, Diethyl malonate 108-59-8, Dimethyl malonate 126-39-6, 2-Butanone ethyleneketal 609-02-9, Dimethyl methylmalonate **930-30-3**, 2-Cyclopentenone **930-68-7**, 2-Cyclohexenone **1121-66-0**, 2-Cycloheptenone **22748-16-9**, 4,4-Dimethyl-2-cyclopentenone 24347-58-8, (2R,3R)-2,3-Butanediol 67421-02-7 167316-27-0
RL: RCT (Reactant); **RACT (Reactant or reagent)**
(process and catalysts for producing optically active cycloalkylmalonates)
IT **151600-50-9P 287493-82-7P 724774-83-8P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(process and catalysts for producing optically active cycloalkylmalonates)
IT **154194-50-0P 160115-23-1P 164931-77-5P 164931-78-6P 173837-41-7P 193530-87-9P 194095-90-4P 287493-81-6P 568590-07-8P 569342-29-6P 724774-82-7P**, 3-[1,1-Bis(methoxycarbonyl)ethyl]cyclopentanone **724774-84-9P**, 3-[(Acetyl)(methoxycarbonyl)methyl]cyclopentanone
RL: SPN (Synthetic preparation); PREP (Preparation)
(process and catalysts for producing optically active cycloalkylmalonates)

L93 ANSWER 3 OF 34 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2004:278187 HCAPLUS
DOCUMENT NUMBER: 141:71293
TITLE: Asymmetric Michael reactions of α-substituted acetates with cyclic enones catalyzed by multifunctional chiral Ru amido complexes
AUTHOR(S): Ikariya, Takao; Wang, Hui; Watanabe, Masahito; Murata, Kunihiko
CORPORATE SOURCE: Graduate School of Science and Engineering, Department of Applied Chemistry, Tokyo Institute of Technology and Frontier Collaborative Research Center, Meguro-ku, Tokyo, 152-8552, Japan
SOURCE: Journal of Organometallic Chemistry (2004), 689(8), 1377-1381

CODEN: JORCAI; ISSN: 0022-328X
PUBLISHER: Elsevier Science B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 141:71293

AB Well-defined 16-electron chiral Ru amido complexes, Ru[(R,R)-diamine](η6-arene), efficiently catalyze asym. Michael addns. of Michael donors to cyclic enones to give adducts in high yields and with excellent ee's. β-Keto esters or nitroacetate as Michael donors react with 2-cyclopentenone in toluene or Me3COH containing the Ru amido catalyst (S/C = 50) to afford the Michael adduct in 99% yield and with up to 92% ee. The outcome of the reaction was delicately influenced by the structures of the diamine and arene ligands as well as reaction conditions.

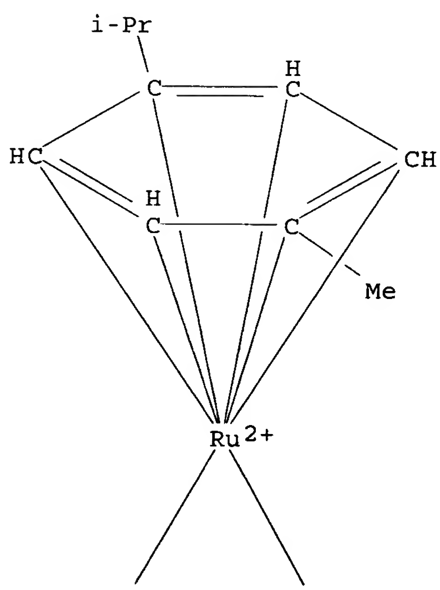
ED Entered STN: 05 Apr 2004

IT **195516-84-8 569336-64-7 569336-66-9**
618912-25-7 709674-02-2 709674-03-3
RL: CAT (Catalyst use); USES (Uses)
(asym. Michael reactions of α-substituted acetates with cyclic enones catalyzed by multifunctional chiral Ru amido complexes)

RN 195516-84-8 HCAPLUS

CN Ruthenium, [N-[(1R,2R)-2-amino-1,2-diphenylethyl]-4-methylbenzenesulfonamidato(2-)-κN][(1,2,3,4,5,6-η)-1-methyl-4-(1-methylethyl)benzene]- (9CI) (CA INDEX NAME)

PAGE 1-A



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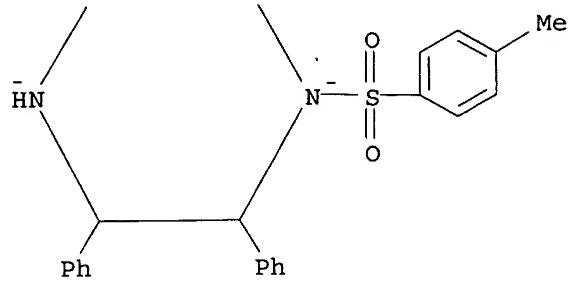
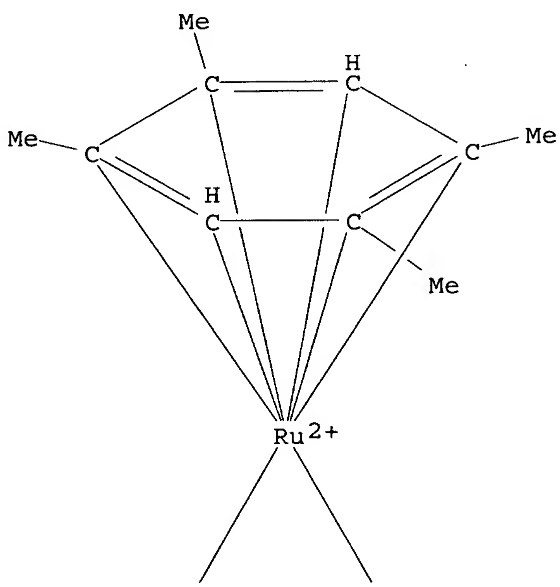


RN 569336-64-7 HCAPLUS
CN Ruthenium, [N-[(1R,2R)-2-(amino-κN)-1,2-diphenylethyl]-4-methylbenzenesulfonamidato(2-)-κN][(1,2,3,4,5,6-η)-1,2,4,5-tetramethylbenzene]- (9CI) (CA INDEX NAME)

PAGE 1-A



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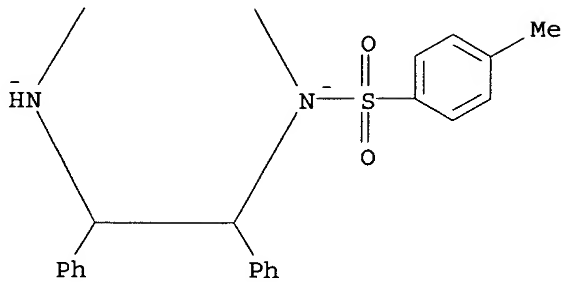
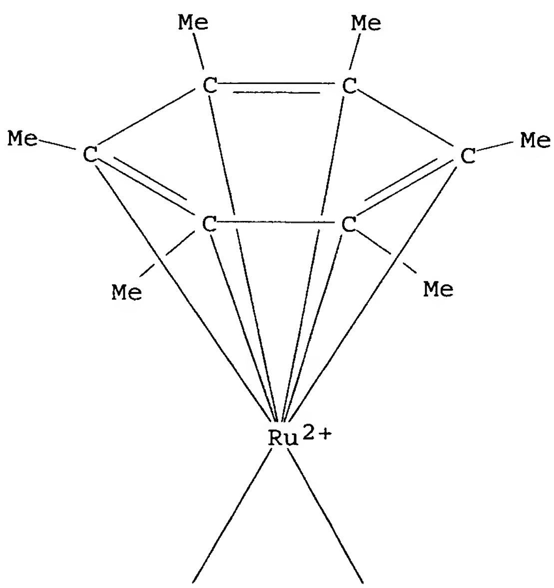


RN 569336-66-9 HCAPLUS
CN Ruthenium, [N-[(1R,2R)-2-(amino-κN)-1,2-diphenylethyl]-4-methylbenzenesulfonamidato(2-)-κN][(1,2,3,4,5,6-η)-hexamethylbenzene]- (9CI) (CA INDEX NAME)

PAGE 1-A



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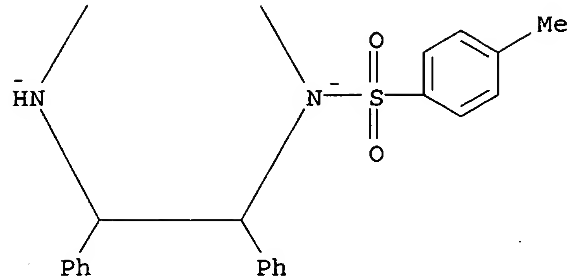

RN 618912-25-7 HCAPLUS
CN Ruthenium, [N-[(1R,2R)-2-amino-1,2-diphenylethyl]methanesulfonamidato(2-)-κN][(1,2,3,4,5,6-η)-hexamethylbenzene]- (9CI)
(CA INDEX NAME)

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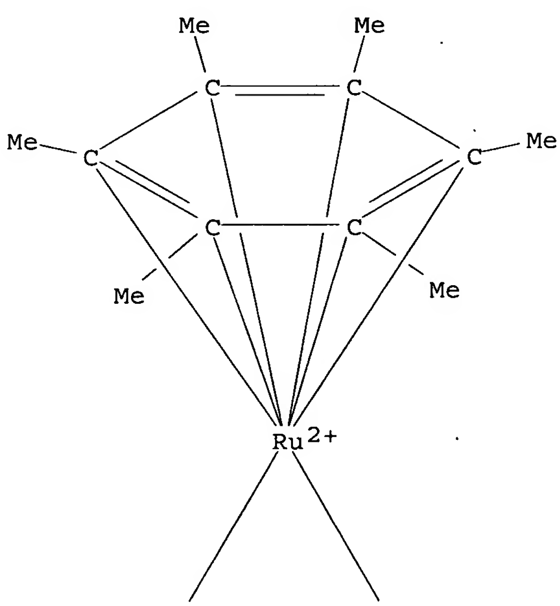
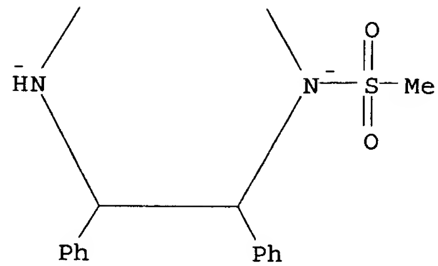
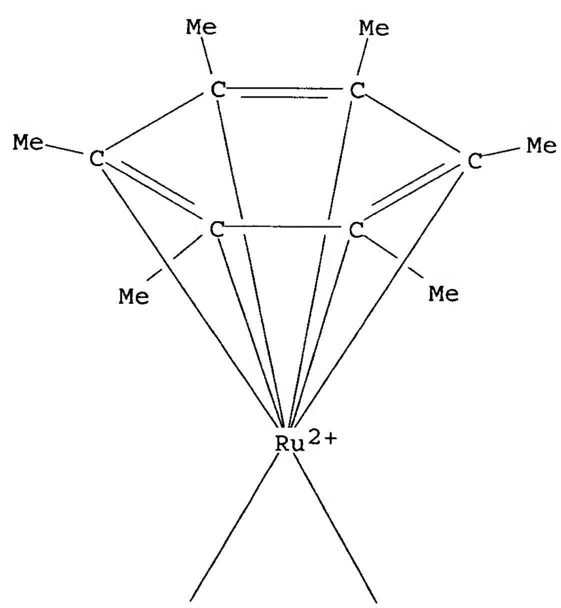


PAGE 2-A



RN 709674-02-2 HCAPLUS
CN Ruthenium, [N-[(1R,2R)-2-(amino-κN)-1,2-diphenylethyl]-1,1,1-trifluoromethanesulfonamidato(2-)-κN][(1,2,3,4,5,6-η)-hexamethylbenzene]- (9CI) (CA INDEX NAME)

PAGE 1-A



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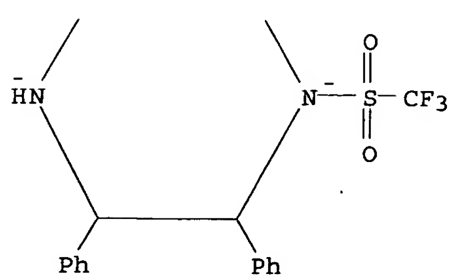
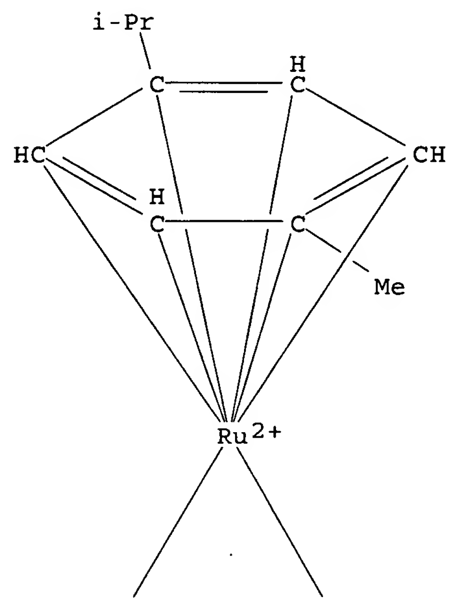
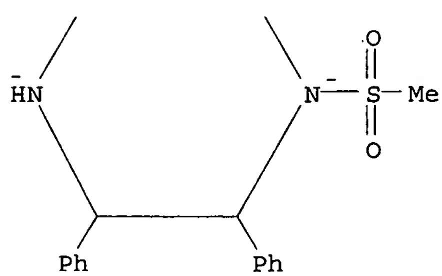


RN 709674-03-3 HCAPLUS
CN Ruthenium, [N-[(1R,2R)-2-(amino-κN)-1,2-diphenylethyl]methanesulfonamidato(2-)-κN][(1,2,3,4,5,6-η)-1-methyl-4-(1-methylethyl)benzene]- (9CI) (CA INDEX NAME)

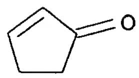
PAGE 1-A



PAGE 2-A



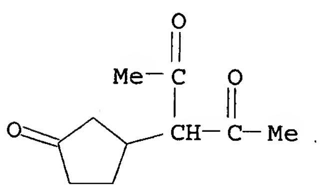
IT **930-30-3**, 2-Cyclopenten-1-one
RL: RCT (Reactant); **RACT (Reactant or reagent)**
(asym. Michael reactions of α-substituted acetates with cyclic enones catalyzed by multifunctional chiral Ru amido complexes)
RN 930-30-3 HCAPLUS
CN 2-Cyclopenten-1-one (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



IT 94410-50-1P 160115-23-1P 646038-06-4P
708266-26-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(asym. Michael reactions of α-substituted acetates with cyclic enones catalyzed by multifunctional chiral Ru amido complexes)

RN 94410-50-1 HCAPLUS

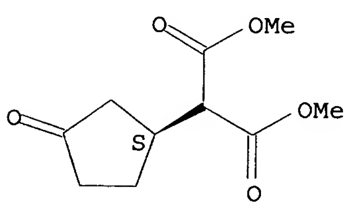
CN 2,4-Pentanedione, 3-(3-oxocyclopentyl)- (9CI) (CA INDEX NAME)



RN 160115-23-1 HCAPLUS

CN Propanedioic acid, [(1S)-3-oxocyclopentyl]-, dimethyl ester (9CI) (CA INDEX NAME)

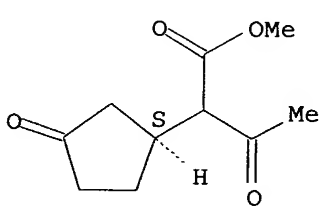
Absolute stereochemistry. Rotation (-).



RN 646038-06-4 HCAPLUS

CN Cyclopentaneacetic acid, α-acetyl-3-oxo-, methyl ester, (1S)- (9CI) (CA INDEX NAME)

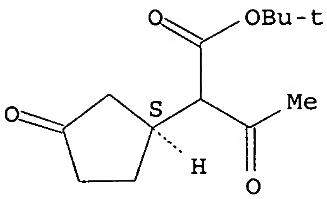
Absolute stereochemistry.



RN 708266-26-6 HCAPLUS

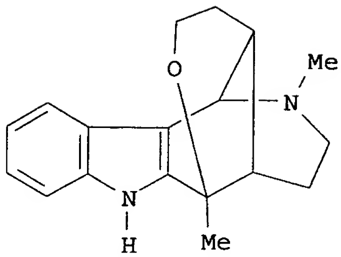
CN Cyclopentaneacetic acid, α-acetyl-3-oxo-, 1,1-dimethylethyl ester, (1S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

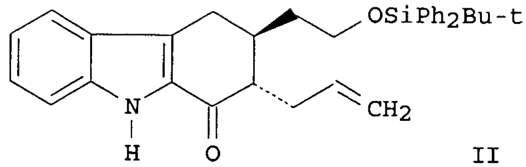


CC 24-4 (Alicyclic Compounds)
IT **Asymmetric synthesis and induction**
(asym. Michael reactions of α-substituted acetates with cyclic enones catalyzed by multifunctional chiral Ru amido complexes)
IT **Michael reaction**
Michael reaction catalysts
(stereoselective; asym. Michael reactions of α-substituted acetates with cyclic enones catalyzed by multifunctional chiral Ru amido complexes)
IT **195516-84-8 569336-64-7 569336-66-9 618912-25-7 709674-02-2 709674-03-3**
RL: CAT (Catalyst use); USES (Uses)
(asym. Michael reactions of α-substituted acetates with cyclic enones catalyzed by multifunctional chiral Ru amido complexes)
IT 105-34-0, Methyl cyanoacetate 105-45-3, Methyl acetoacetate 108-59-8, Dimethyl malonate 123-54-6, Acetylacetone, reactions 626-35-7, Ethyl nitroacetate **930-30-3**, 2-Cyclopenten-1-one 1694-31-1, tert-Butyl acetoacetate
RL: RCT (Reactant); **RACT (Reactant or reagent)**
(asym. Michael reactions of α-substituted acetates with cyclic enones catalyzed by multifunctional chiral Ru amido complexes)
IT **94410-50-1P 160115-23-1P 646038-06-4P 708266-26-6P** 708266-27-7P 708266-28-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(asym. Michael reactions of α-substituted acetates with cyclic enones catalyzed by multifunctional chiral Ru amido complexes)
REFERENCE COUNT: 37 THERE ARE 37 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L93 ANSWER 4 OF 34 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2004:168607 HCAPLUS
DOCUMENT NUMBER: 140:357534
TITLE: Enantioselective Synthesis of (-)-Gilbertine via a Cationic Cascade Cyclization
AUTHOR(S): Jiricek, Jan; Blechert, Siegfried
CORPORATE SOURCE: Institut fuer Chemie, Technische Universitaet Berlin, Berlin, 10623, Germany
SOURCE: Journal of the American Chemical Society (**2004**), 126(11), 3534-3538
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 140:357534
GI



I



II

AB Described is the first enantioselective synthesis of (-)-gilbertine (I), a member of the uleine-type family, and the determination of the absolute configuration of this natural product is reported. The key step employs a cationic cascade reaction for a tetrahydropyran and piperidine ring formation and the construction of the pentacyclic framework in one step. The synthetic strategy utilizes the Shibasaki reaction to build up the first stereogenic center. A formylation reaction of a 3-substituted cyclohexanone derivative was achieved, giving only the desired regioisomer. The Japp-Klingemann Fischer indole protocol was used successfully as a convergent synthetic approach for the construction of the desired tetrahydrocarbazole (II). Furthermore, an unexpected behavior of this 2,3-disubstituted cyclohexanone derivative during an epimerization process was investigated, resulting in different chemical behavior of the enantiomers and the racemate. The diastereomeric resolution was achieved via the cationic cascade reaction, demonstrating the versatility of this approach. Significantly, the synthetic 17-step sequence was easy to execute, giving (-)-gilbertine in 5.5% overall yield.

ED Entered STN: 02 Mar 2004

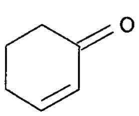
IT **930-68-7**, 2-Cyclohexen-1-one

RL: RCT (Reactant); **RACT (Reactant or reagent)**

(enantioselective synthesis of (-)-gilbertine via a cationic cascade cyclization)

RN 930-68-7 HCAPLUS

CN 2-Cyclohexen-1-one (6CI, 8CI, 9CI) (CA INDEX NAME)



IT **164931-77-5P 619329-97-4P**

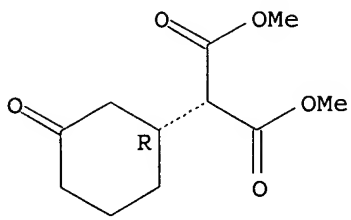
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(enantioselective synthesis of (-)-gilbertine via a cationic cascade cyclization)

RN 164931-77-5 HCAPLUS

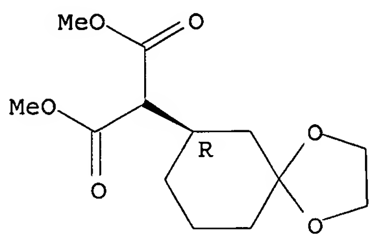
CN Propanedioic acid, [(1R)-3-oxocyclohexyl]-, dimethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



RN 619329-97-4 HCAPLUS
CN Propanedioic acid, (7R)-1,4-dioxaspiro[4.5]dec-7-yl-, dimethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



CC 31-5 (Alkaloids)
IT **Asymmetric synthesis and induction**
(enantioselective synthesis of (-)-gilbertine via a cationic cascade cyclization)
IT 62-53-3, Aniline, reactions 106-95-6, Allyl bromide, reactions 108-59-8, Dimethyl malonate 109-94-4, Ethyl formate **930-68-7**, 2-Cyclohexen-1-one 4229-44-1, N-Methylhydroxylamine hydrochloride 681280-81-9
RL: RCT (Reactant); **RACT (Reactant or reagent)**
(enantioselective synthesis of (-)-gilbertine via a cationic cascade cyclization)
IT 71366-23-9P 85783-97-7P **164931-77-5P**
619329-97-4P 681280-63-7P 681280-64-8P 681280-65-9P
681280-66-0P 681280-67-1P 681280-68-2P 681280-71-7P
681280-72-8P 681280-73-9P 681280-74-0P 681280-75-1P
681280-76-2P 681280-78-4P 681280-79-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(enantioselective synthesis of (-)-gilbertine via a cationic cascade cyclization)
REFERENCE COUNT: 34 THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L93 ANSWER 5 OF 34 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2003:707973 HCAPLUS
DOCUMENT NUMBER: 139:307538
TITLE: Fe3+-exchanged fluorotetrasilicic mica as an active and reusable catalyst for the Michael reaction
AUTHOR(S): Shimizu, Ken-ichi; Miyagi, Masato; Kan-no, Toshiki; Kodama, Tatsuya; Kitayama, Yoshie
CORPORATE SOURCE: Graduate School of Science and Technology,

Niigata University, Niigata, 950-2181, Japan

SOURCE: Tetrahedron Letters (**2003**), 44(40), 7421-7424
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier Science B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 139:307538

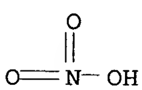
AB Fe3+-exchanged fluorotetrasilicic mica acts as a highly effective and reusable catalyst for the solventless Michael reaction of β-ketoesters with vinyl ketones under mild conditions. The immobilized catalyst shows higher activity than homogeneous Fe3+ catalysts, FeCl3·6H2O and Fe(NO3)3·9H2O.

ED Entered STN: 10 Sep 2003

IT **7782-61-8**, Ferric nitrate nonahydrate
RL: CAT (Catalyst use); USES (Uses)
(iron(3+)-exchanged fluorotetrasilicic mica as catalyst for Michael reaction of oxo esters with vinyl ketones)

RN 7782-61-8 HCAPLUS

CN Nitric acid, iron(3+) salt, nonahydrate (9CI) (CA INDEX NAME)



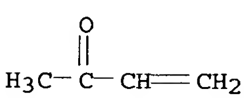
●1/3 Fe(III)

●3 H_2O

IT **78-94-4**, 3-Buten-2-one, reactions **1629-58-9**, Ethyl vinyl ketone
RL: RCT (Reactant); RACT (Reactant or reagent)
(iron(3+)-exchanged fluorotetrasilicic mica as catalyst for Michael reaction of oxo esters with vinyl ketones)

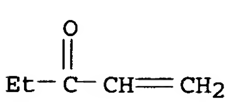
RN 78-94-4 HCAPLUS

CN 3-Buten-2-one (8CI, 9CI) (CA INDEX NAME)



RN 1629-58-9 HCAPLUS

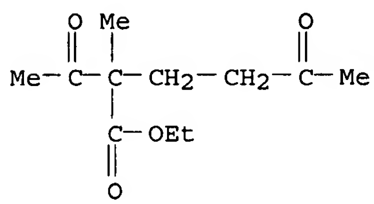
CN 1-Penten-3-one (7CI, 8CI, 9CI) (CA INDEX NAME)



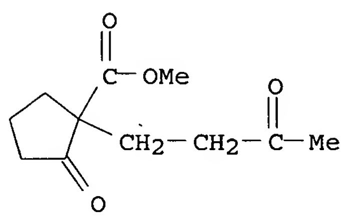
IT **28793-08-0P 31208-52-3P 35490-05-2P**

61771-80-0P 61771-81-1P 176101-58-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(iron(3+)-exchanged fluorotetrasilicic mica as catalyst for Michael reaction of oxo esters with vinyl ketones)

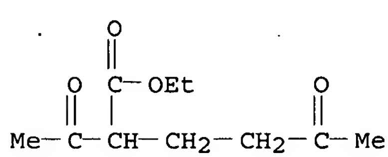
RN 28793-08-0 HCAPLUS
CN Hexanoic acid, 2-acetyl-2-methyl-5-oxo-, ethyl ester (6CI, 8CI, 9CI) (CA INDEX NAME)



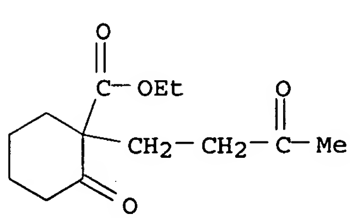
RN 31208-52-3 HCAPLUS
CN Cyclopentanecarboxylic acid, 2-oxo-1-(3-oxobutyl)-, methyl ester (8CI, 9CI) (CA INDEX NAME)



RN 35490-05-2 HCAPLUS
CN Hexanoic acid, 2-acetyl-5-oxo-, ethyl ester (6CI, 7CI, 9CI) (CA INDEX NAME)

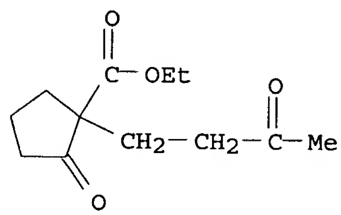


RN 61771-80-0 HCAPLUS
CN Cyclohexanecarboxylic acid, 2-oxo-1-(3-oxobutyl)-, ethyl ester (7CI, 9CI) (CA INDEX NAME)

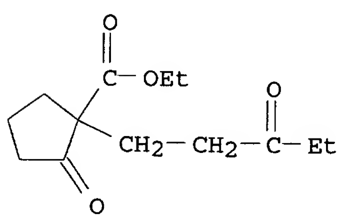


RN 61771-81-1 HCAPLUS

CN Cyclopentanecarboxylic acid, 2-oxo-1-(3-oxobutyl)-, ethyl ester (6CI, 7CI, 9CI) (CA INDEX NAME)



RN 176101-58-9 HCAPLUS
CN Cyclopentanecarboxylic acid, 2-oxo-1-(3-oxopentyl)-, ethyl ester (9CI) (CA INDEX NAME)



CC 24-4 (Alicyclic Compounds)
Section cross-reference(s): 23
IT **Michael reaction catalysts**
(iron(3+)-exchanged fluorotetrasilicic mica as catalyst for Michael reaction of oxo esters with vinyl ketones)
IT 1318-93-0, Montmorillonite ((Al1.33-1.67Mg0.33-0.67)(Ca0-1Na0-1)0.33Si4(OH)2O10.xH2O), uses **7782-61-8**, Ferric nitrate nonahydrate 10025-77-1, Ferric chloride hexahydrate 20074-52-6, Iron(3+), uses 56450-90-9, Fluorotetrasilicic mica
RL: CAT (Catalyst use); USES (Uses)
(iron(3+)-exchanged fluorotetrasilicic mica as catalyst for Michael reaction of oxo esters with vinyl ketones)
IT **78-94-4**, 3-Buten-2-one, reactions 141-97-9, Ethyl acetoacetate 609-14-3, Ethyl 2-methylacetoacetate 611-10-9 **1629-58-9**, Ethyl vinyl ketone 1655-07-8 10472-24-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(iron(3+)-exchanged fluorotetrasilicic mica as catalyst for Michael reaction of oxo esters with vinyl ketones)
IT **28793-08-0P 31208-52-3P 35490-05-2P 61771-80-0P 61771-81-1P 176101-58-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(iron(3+)-exchanged fluorotetrasilicic mica as catalyst for Michael reaction of oxo esters with vinyl ketones)
REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L93 ANSWER 6 OF 34 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2003:406901 HCAPLUS
DOCUMENT NUMBER: 139:133131
TITLE: Enantioselective Michael Reaction Catalyzed by

Well-Defined Chiral Ru Amido Complexes: Isolation and Characterization of the Catalyst Intermediate, Ru Malonato Complex Having a Metal-Carbon Bond

AUTHOR(S): Watanabe, Masahito; Murata, Kunihiko; Ikariya, Takao
CORPORATE SOURCE: Department of Applied Chemistry, Graduate School of Science and Engineering, Tokyo Institute of Technology and Frontier Collaborative Research Center, Tokyo, 152-8552, Japan

SOURCE: Journal of the American Chemical Society (**2003**), 125(25), 7508-7509
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 139:133131

AB Chiral Ru amido complexes promote asym. Michael addition of malonates to cyclic enones, leading to Michael adducts with excellent ee's, in which the chiral Ru amido complexes react with malonates to give isolable catalyst intermediates, chiral Ru malonato complexes bearing a metal bound C-nucleophile.

ED Entered STN: 29 May 2003

IT **569336-67-0**

RL: CPS (Chemical process); FMU (Formation, unclassified); PEP (Physical, engineering or chemical process); RCT (Reactant); FORM (Formation, nonpreparative); PROC (Process); RACT (Reactant or reagent)

(crystal structure of; enantioselective Michael reaction catalyzed by well-defined chiral Ru amido complexes and isolation and Ru malonato complex having metal-carbon bond catalyst intermediate characterization)

RN 569336-67-0 HCAPLUS

CN Ruthenium, [N-[(1R,2R)-2-(amino-κN)-1,2-diphenylethyl]-4-methylbenzenesulfonamidato-κN][2-methoxy-1-(methoxycarbonyl)-2-oxoethyl][(1,2,3,4,5,6-η)-1,3,5-trimethylbenzene]- (9CI) (CA INDEX NAME)

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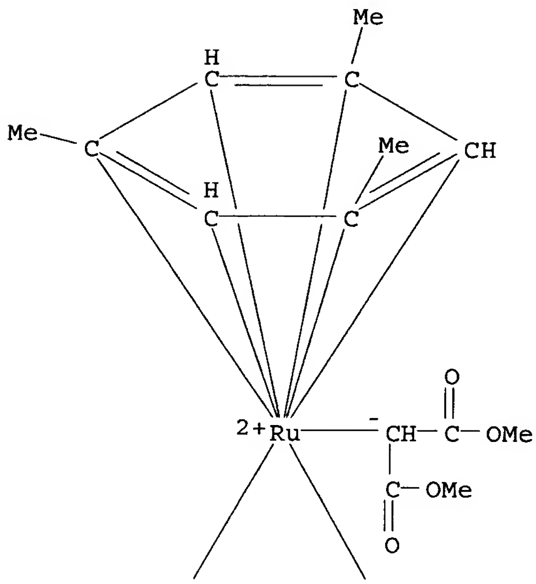

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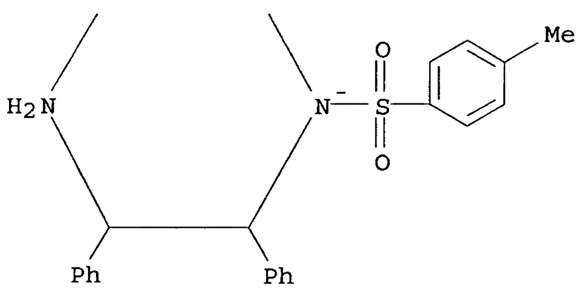

IT 195516-84-8 569336-63-6 569336-64-7
569336-65-8 569336-66-9 618912-25-7
RL: CAT (Catalyst use); CPS (Chemical process); PEP (Physical, engineering or chemical process); RCT (Reactant); PROC (Process); RACT (Reactant or reagent); USES (Uses)
(enantioselective Michael reaction catalyzed by well-defined chiral Ru amido complexes and isolation and Ru malonato complex having metal-carbon bond catalyst intermediate characterization)

RN 195516-84-8 HCAPLUS

CN Ruthenium, [N-[(1R,2R)-2-amino-1,2-diphenylethyl]-4-methylbenzenesulfonamidato(2-)-κN][(1,2,3,4,5,6-η)-1-methyl-4-(1-methylethyl)benzene]- (9CI) (CA INDEX NAME)

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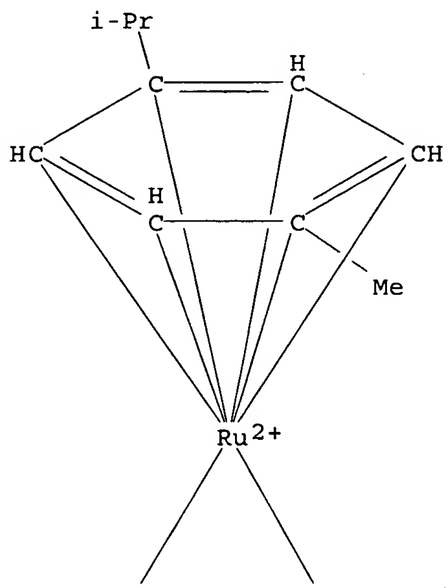

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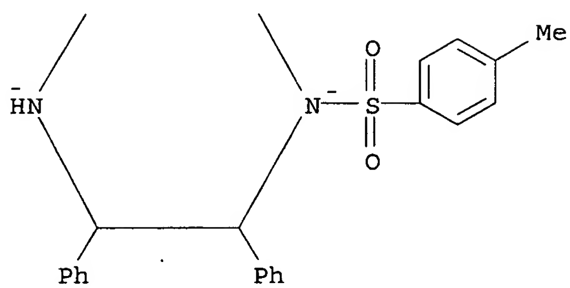

RN 569336-63-6 HCAPLUS
CN Ruthenium, [N-[(1R,2R)-2-(amino-κN)-1,2-diphenylethyl]-4-methylbenzenesulfonamidato(2-)-κN][(1,2,3,4,5,6-η)-1,3,5-trimethylbenzene]- (9CI) (CA INDEX NAME)

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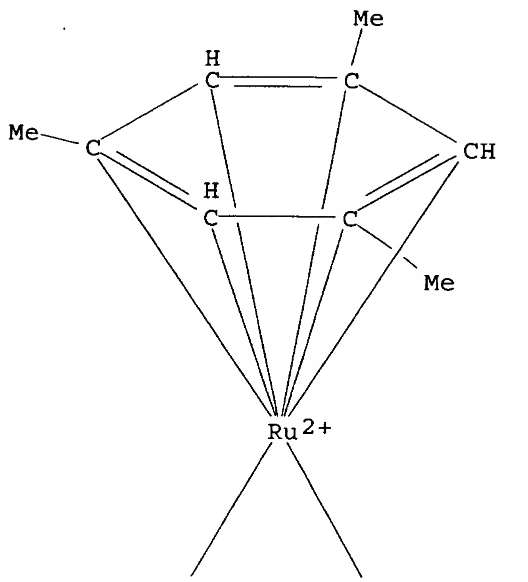

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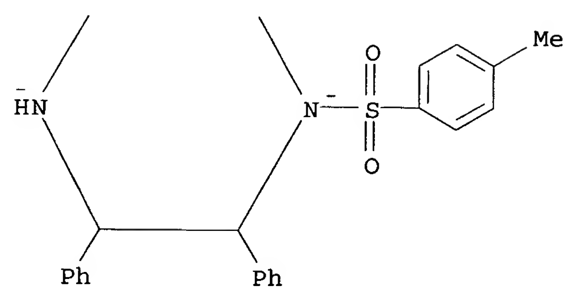
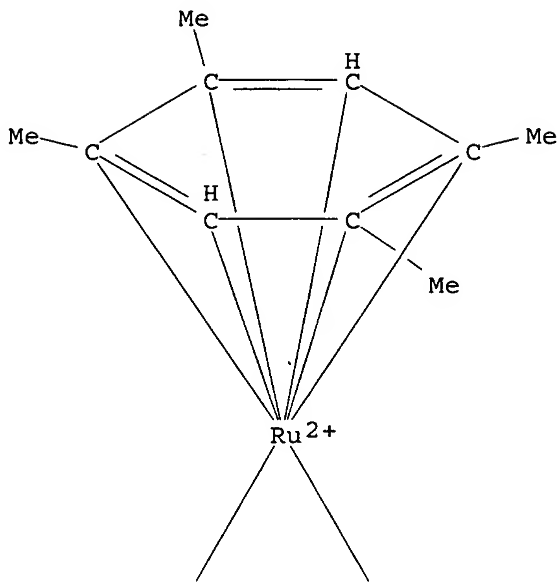


RN 569336-64-7 HCAPLUS
CN Ruthenium, [N-[(1R,2R)-2-(amino-κN)-1,2-diphenylethyl]-4-methylbenzenesulfonamidato(2-)-κN][(1,2,3,4,5,6-η)-1,2,4,5-tetramethylbenzene]- (9CI) (CA INDEX NAME)

PAGE 1-A



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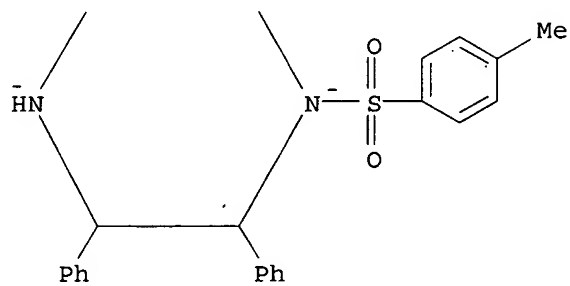
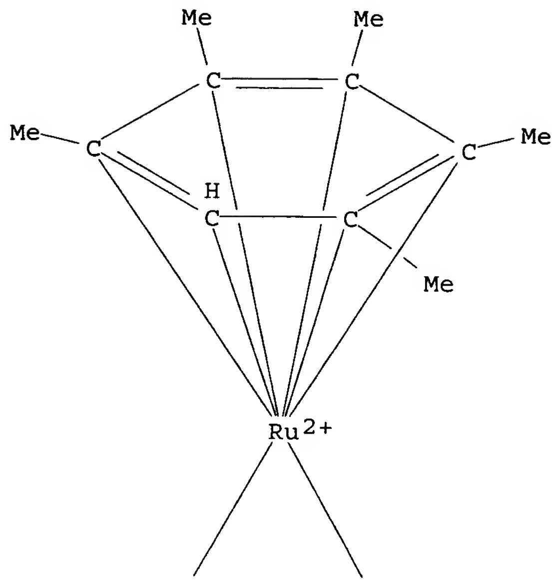
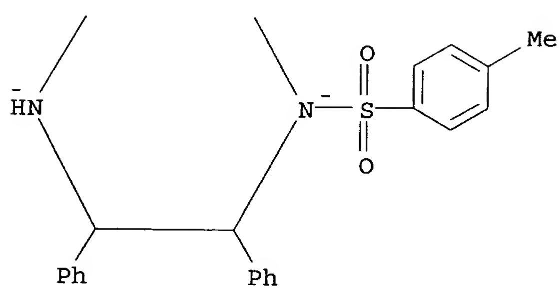


RN 569336-65-8 HCAPLUS
CN Ruthenium, [N-[(1R,2R)-2-(amino-κN)-1,2-diphenylethyl]-4-methylbenzenesulfonamidato(2-)-κN][(1,2,3,4,5,6-η)-pentamethylbenzene]- (9CI) (CA INDEX NAME)

PAGE 1-A

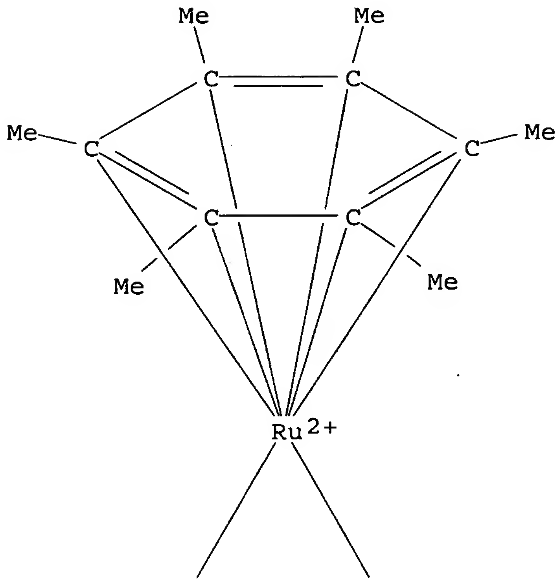


PAGE 2-A



RN 569336-66-9 HCAPLUS
CN Ruthenium, [N-[(1R,2R)-2-(amino-κN)-1,2-diphenylethyl]-4-methylbenzenesulfonamidato(2-)-κN][(1,2,3,4,5,6-η)-hexamethylbenzene]- (9CI) (CA INDEX NAME)

PAGE 1-A



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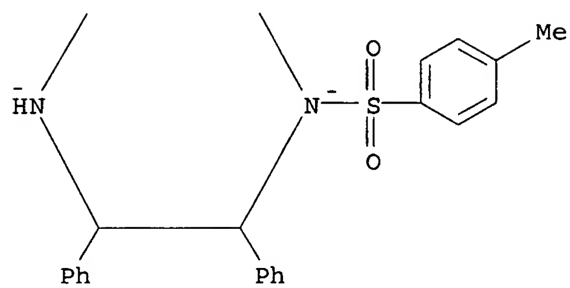
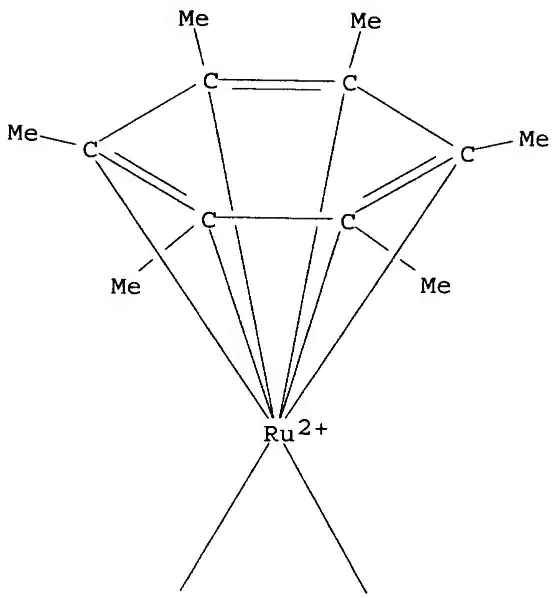
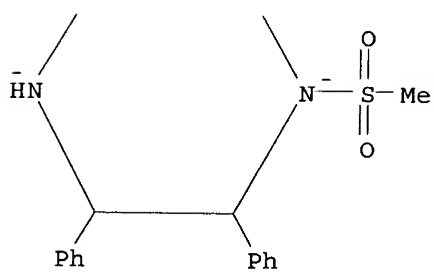


RN 618912-25-7 HCAPLUS
CN Ruthenium, [N-[(1R,2R)-2-amino-1,2-diphenylethyl]methanesulfonamid
ato(2-)-κN][(1,2,3,4,5,6-η)-hexamethylbenzene]- (9CI)
(CA INDEX NAME)

PAGE 1-A

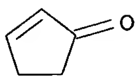


PAGE 2-A

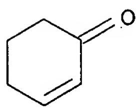


IT 930-30-3, 2-Cyclopentenone **930-68-7**, 2-Cyclohexenone **1121-66-0**, 2-Cycloheptenone **22748-16-9**, 4,4-Dimethyl-2-cyclopentenone
RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); RCT (Reactant); PROC (Process); **RACT (Reactant or reagent)**
(enantioselective Michael reaction catalyzed by well-defined chiral Ru amido complexes and isolation and Ru malonato complex having metal-carbon bond catalyst intermediate characterization)

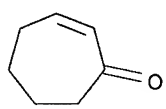
RN 930-30-3 HCAPLUS
CN 2-Cyclopenten-1-one (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



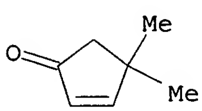
RN 930-68-7 HCAPLUS
CN 2-Cyclohexen-1-one (6CI, 8CI, 9CI) (CA INDEX NAME)



RN 1121-66-0 HCAPLUS
CN 2-Cyclohepten-1-one (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

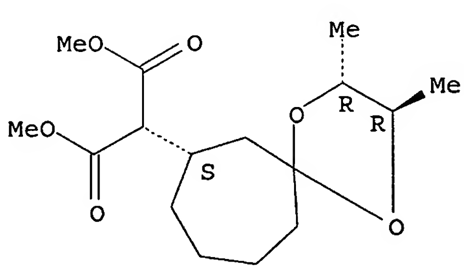


RN 22748-16-9 HCAPLUS
CN 2-Cyclopenten-1-one, 4,4-dimethyl- (7CI, 8CI, 9CI) (CA INDEX NAME)



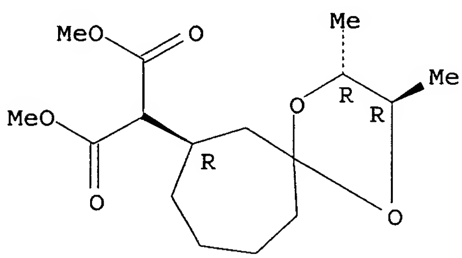
IT **569342-28-5 569342-29-6**
RL: FMU (Formation, unclassified); FORM (Formation, nonpreparative)
(enantioselective Michael reaction catalyzed by well-defined chiral Ru amido complexes and isolation and Ru malonato complex having metal-carbon bond catalyst intermediate characterization)
RN 569342-28-5 HCAPLUS
CN Propanedioic acid, [(2R,3R,7S)-2,3-dimethyl-1,4-dioxaspiro[4.6]undec-7-yl]-, dimethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



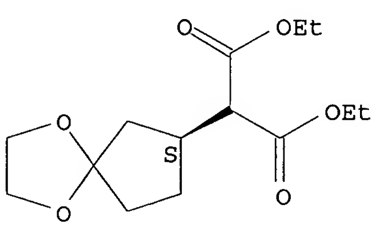
RN 569342-29-6 HCAPLUS
CN Propanedioic acid, [(2R,3R,7R)-2,3-dimethyl-1,4-dioxaspiro[4.6]undec-7-yl]-, dimethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

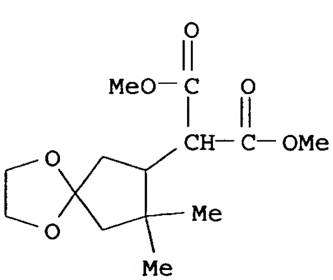


IT **193530-88-0 568590-07-8**
RL: FMU (Formation, unclassified); PEP (Physical, engineering or chemical process); PYP (Physical process); FORM (Formation, nonpreparative); PROC (Process)
(enantioselective Michael reaction catalyzed by well-defined chiral Ru amido complexes and isolation and Ru malonato complex having metal-carbon bond catalyst intermediate characterization)
RN 193530-88-0 HCAPLUS
CN Propanedioic acid, (7S)-1,4-dioxaspiro[4.4]non-7-yl-, diethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



RN 568590-07-8 HCAPLUS
CN Propanedioic acid, (8,8-dimethyl-1,4-dioxaspiro[4.4]non-7-yl)-, dimethyl ester (9CI) (CA INDEX NAME)



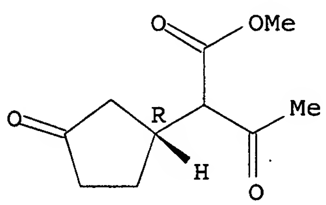
IT **568590-08-9P**

RL: PEP (Physical, engineering or chemical process); PYP (Physical process); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); PROC (Process); RACT (Reactant or reagent)
(enantioselective Michael reaction catalyzed by well-defined chiral Ru amido complexes and isolation and Ru malonato complex having metal-carbon bond catalyst intermediate characterization)

RN 568590-08-9 HCAPLUS

CN Cyclopentaneacetic acid, α-acetyl-3-oxo-, methyl ester, (1R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

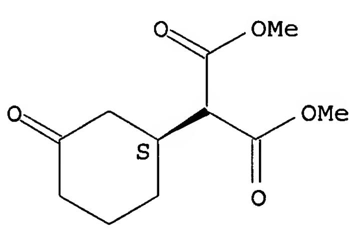


IT **154194-50-0P 160115-23-1P 568590-05-6P**
RL: PEP (Physical, engineering or chemical process); PYP (Physical process); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)
(enantioselective Michael reaction catalyzed by well-defined chiral Ru amido complexes and isolation and Ru malonato complex having metal-carbon bond catalyst intermediate characterization)

RN 154194-50-0 HCAPLUS

CN Propanedioic acid, [(1S)-3-oxocyclohexyl]-, dimethyl ester (9CI) (CA INDEX NAME)

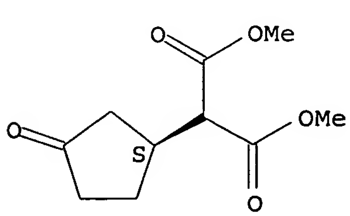
Absolute stereochemistry. Rotation (-).



RN 160115-23-1 HCAPLUS

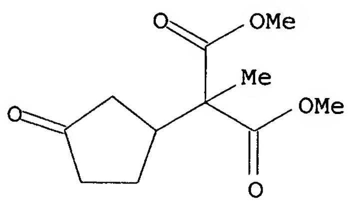
CN Propanedioic acid, [(1S)-3-oxocyclopentyl]-, dimethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



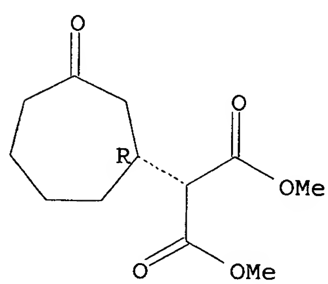
RN 568590-05-6 HCAPLUS
CN Propanedioic acid, methyl(3-oxocyclopentyl)-, dimethyl ester, (-)-
(9CI) (CA INDEX NAME)

Rotation (-).



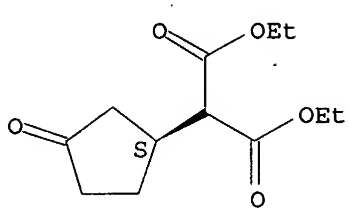
IT **287493-82-7**
RL: RCT (Reactant); RACT (Reactant or reagent)
(enantioselective Michael reaction catalyzed by well-defined chiral Ru amido complexes and isolation and Ru malonato complex having metal-carbon bond catalyst intermediate characterization)
RN 287493-82-7 HCAPLUS
CN Propanedioic acid, [(1R)-3-oxocycloheptyl]-, dimethyl ester (9CI)
(CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



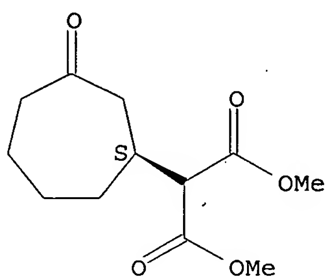
IT **193530-87-9P 568590-04-5P 568590-06-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(enantioselective Michael reaction catalyzed by well-defined chiral Ru amido complexes and isolation and Ru malonato complex having metal-carbon bond catalyst intermediate characterization)
RN 193530-87-9 HCAPLUS
CN Propanedioic acid, [(1S)-3-oxocyclopentyl]-, diethyl ester (9CI)
(CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



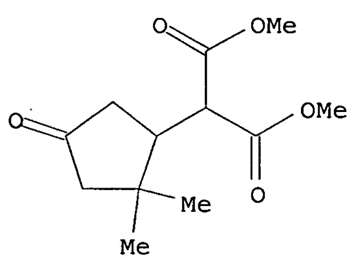
RN 568590-04-5 HCAPLUS
CN Propanedioic acid, [(1S)-3-oxocycloheptyl]-, dimethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 568590-06-7 HCAPLUS
CN Propanedioic acid, (2,2-dimethyl-4-oxocyclopentyl)-, dimethyl ester, (-)- (9CI) (CA INDEX NAME)

Rotation (-).



CC 22-3 (Physical Organic Chemistry)
Section cross-reference(s): 29, 75
IT **Asymmetric synthesis and induction**
Stereochemistry
Transition state structure
(enantioselective Michael reaction catalyzed by well-defined chiral Ru amido complexes and isolation and Ru malonato complex having metal-carbon bond catalyst intermediate characterization)
IT **Michael reaction**
Michael reaction catalysts
(stereoselective; enantioselective Michael reaction catalyzed by well-defined chiral Ru amido complexes and isolation and Ru malonato complex having metal-carbon bond catalyst intermediate characterization)

IT **569336-67-0**
RL: CPS (Chemical process); FMU (Formation, unclassified); PEP (Physical, engineering or chemical process); RCT (Reactant); FORM (Formation, nonpreparative); PROC (Process); RACT (Reactant or reagent)
(crystal structure of; enantioselective Michael reaction catalyzed by well-defined chiral Ru amido complexes and isolation and Ru malonato complex having metal-carbon bond catalyst intermediate characterization)

IT **195516-84-8 569336-63-6 569336-64-7 569336-65-8 569336-66-9 618912-25-7**
RL: CAT (Catalyst use); CPS (Chemical process); PEP (Physical, engineering or chemical process); RCT (Reactant); PROC (Process); RACT (Reactant or reagent); USES (Uses)
(enantioselective Michael reaction catalyzed by well-defined chiral Ru amido complexes and isolation and Ru malonato complex having metal-carbon bond catalyst intermediate characterization)

IT 105-45-3, Methyl acetylacetate 105-53-3, Diethyl malonate 108-59-8, Dimethyl malonate 609-02-9, Dimethyl methylmalonate **930-30-3**, 2-Cyclopentenone **930-68-7**, 2-Cyclohexenone **1121-66-0**, 2-Cycloheptenone **22748-16-9**, 4,4-Dimethyl-2-cyclopentenone
RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); RCT (Reactant); PROC (Process); **RACT (Reactant or reagent)**
(enantioselective Michael reaction catalyzed by well-defined chiral Ru amido complexes and isolation and Ru malonato complex having metal-carbon bond catalyst intermediate characterization)

IT 84308-31-6 **569342-28-5 569342-29-6**
RL: FMU (Formation, unclassified); FORM (Formation, nonpreparative)
(enantioselective Michael reaction catalyzed by well-defined chiral Ru amido complexes and isolation and Ru malonato complex having metal-carbon bond catalyst intermediate characterization)

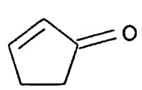
IT **193530-88-0 568590-07-8**
RL: FMU (Formation, unclassified); PEP (Physical, engineering or chemical process); PYP (Physical process); FORM (Formation, nonpreparative); PROC (Process)
(enantioselective Michael reaction catalyzed by well-defined chiral Ru amido complexes and isolation and Ru malonato complex having metal-carbon bond catalyst intermediate characterization)

IT **568590-08-9P**
RL: PEP (Physical, engineering or chemical process); PYP (Physical process); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); PROC (Process); RACT (Reactant or reagent)
(enantioselective Michael reaction catalyzed by well-defined chiral Ru amido complexes and isolation and Ru malonato complex having metal-carbon bond catalyst intermediate characterization)

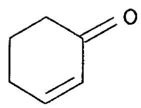
IT **154194-50-0P 160115-23-1P 568590-05-6P**
RL: PEP (Physical, engineering or chemical process); PYP (Physical process); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)
(enantioselective Michael reaction catalyzed by well-defined chiral Ru amido complexes and isolation and Ru malonato complex having metal-carbon bond catalyst intermediate

characterization)
IT 126-39-6, 2-Ethyl-2-methyl-1,3-dioxolane **287493-82-7**
RL: RCT (Reactant); RACT (Reactant or reagent)
(enantioselective Michael reaction catalyzed by well-defined chiral Ru amido complexes and isolation and Ru malonato complex having metal-carbon bond catalyst intermediate characterization)
IT **193530-87-9P 568590-04-5P 568590-06-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(enantioselective Michael reaction catalyzed by well-defined chiral Ru amido complexes and isolation and Ru malonato complex having metal-carbon bond catalyst intermediate characterization)
REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L93 ANSWER 7 OF 34 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2003:315962 HCAPLUS
DOCUMENT NUMBER: 140:76842
TITLE: Effect of microwaves in the chiral switching asymmetric Michael reaction
AUTHOR(S): Narasimhan, S.; Velmathi, S.
CORPORATE SOURCE: Centre for Natural Products, SPIC Science Foundation, Guindy, Chennai, 600 032, India
SOURCE: Molecules **(2003)**, 8(2), 256-262
CODEN: MOLEFW; ISSN: 1420-3049
URL: http://www.mdpi.org/molecules/papers/80200256.pdf
PUBLISHER: Molecular Diversity Preservation International
DOCUMENT TYPE: Journal; (online computer file)
LANGUAGE: English
OTHER SOURCE(S): CASREACT 140:76842
AB Highly enantioselective Michael reactions of malonates with cyclic enones are achieved in remarkably less time under microwave irradiation using newly developed heterobimetallic catalysts.
ED Entered STN: 24 Apr 2003
IT **930-30-3**, 2-Cyclopenten-1-one **930-68-7**, 2-Cyclohexen-1-one
RL: RCT (Reactant); **RACT (Reactant or reagent)**
(enantioselective Michael addition reaction of cyclic enones with malonates utilizing chiral heterobimetallic catalyst system under microwave irradiation)
RN 930-30-3 HCAPLUS
CN 2-Cyclopenten-1-one (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



RN 930-68-7 HCAPLUS
CN 2-Cyclohexen-1-one (6CI, 8CI, 9CI) (CA INDEX NAME)

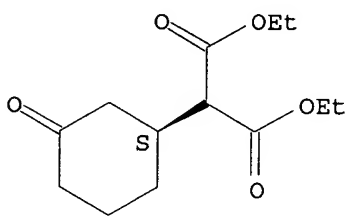


IT 151600-50-9P 164931-78-6P 177722-18-8P
193530-87-9P 334699-04-6P 334699-05-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(enantioselective Michael addition reaction of cyclic enones with malonates utilizing chiral heterobimetallic catalyst system under microwave irradiation)

RN 151600-50-9 HCAPLUS

CN Propanedioic acid, [(1S)-3-oxocyclohexyl]-, diethyl ester (9CI) (CA INDEX NAME)

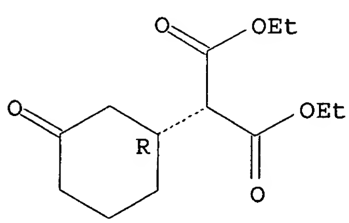
Absolute stereochemistry. Rotation (-).



RN 164931-78-6 HCAPLUS

CN Propanedioic acid, [(1R)-3-oxocyclohexyl]-, diethyl ester (9CI) (CA INDEX NAME)

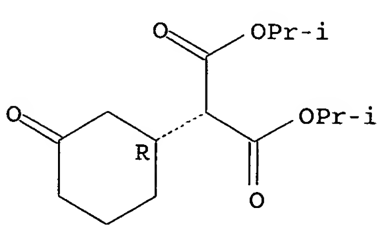
Absolute stereochemistry. Rotation (+).



RN 177722-18-8 HCAPLUS

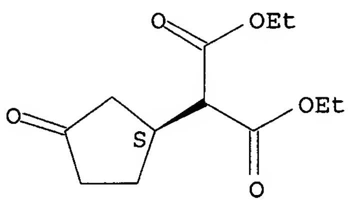
CN Propanedioic acid, [(1R)-3-oxocyclohexyl]-, bis(1-methylethyl) ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



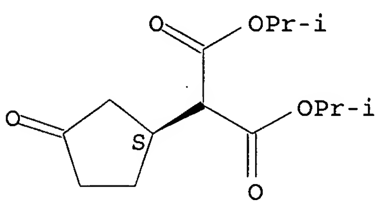
RN 193530-87-9 HCAPLUS
CN Propanedioic acid, [(1S)-3-oxocyclopentyl]-, diethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



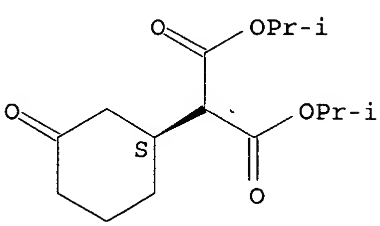
RN 334699-04-6 HCAPLUS
CN Propanedioic acid, [(1S)-3-oxocyclopentyl]-, bis(1-methylethyl) ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



RN 334699-05-7 HCAPLUS
CN Propanedioic acid, [(1S)-3-oxocyclohexyl]-, bis(1-methylethyl) ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



CC 24-5 (Alicyclic Compounds)
Section cross-reference(s): 23
IT **Asymmetric synthesis and induction**
(enantioselective Michael addition reaction of cyclic enones with malonates utilizing chiral heterobimetallic catalyst system under microwave irradiation)
IT Addition reaction catalysts
Michael reaction
(stereoselective; enantioselective Michael addition reaction of cyclic enones with malonates utilizing chiral heterobimetallic catalyst system under microwave irradiation)
IT 105-53-3, Ethyl malonate **930-30-3**, 2-Cyclopenten-1-one **930-68-7**, 2-Cyclohexen-1-one 13195-64-7, Diisopropyl

malonate 15014-25-2, Dibenzyl malonate
RL: RCT (Reactant); **RACT (Reactant or reagent)**
(enantioselective Michael addition reaction of cyclic enones with malonates utilizing chiral heterobimetallic catalyst system under microwave irradiation)

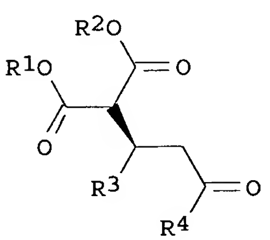
IT **151600-50-9P** 154194-47-5P 154194-49-7P 164931-75-3P
164931-78-6P 177722-18-8P 193530-87-9P
334699-04-6P 334699-05-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(enantioselective Michael addition reaction of cyclic enones with malonates utilizing chiral heterobimetallic catalyst system under microwave irradiation)

REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

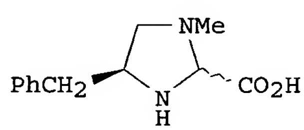
L93 ANSWER 8 OF 34 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2003:160178 HCAPLUS
DOCUMENT NUMBER: 139:36248
TITLE: Highly enantioselective organocatalytic conjugate addition of malonates to acyclic α,β-unsaturated enones
AUTHOR(S): Halland, Nis; Aburel, Pompiliu S.; Jorgensen, Karl Anker
CORPORATE SOURCE: Danish National Research Foundation: Center for Catalysis Department of Chemistry, Aarhus University, Aarhus C, 8000, Den.
SOURCE: Angewandte Chemie, International Edition (**2003**), 42(6), 661-665
CODEN: ACIEF5; ISSN: 1433-7851
PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 139:36248

GI



I



II

AB We have developed the first highly enantioselective selective organocatalytic Michael addition of malonates R1O2CCH2CO2R2 (R1 = R2 = Me, Et, CHMe2, CMe3, allyl, CH2Ph; R1 = CH2Ph, R2 = Me, Et; R1 = Et, R2 = CMe3) to α,β-unsatd. enones R3CH:CHCOR4 [R3 = Ph, 2-naphthyl, 4-ClC6H4, 4-HOC6H4, etc., R4 = Me; R3R4 = (CH2)3; R3 = Ph, R4 = Et, CHMe2] to offer adducts I using an imidazolidine catalyst II easily prepared from phenylalanine. The scope of the reaction is demonstrated by the synthesis of optically active δ keto esters, e.g. Me (3R)-5-oxo-3-phenylhexanoate, and

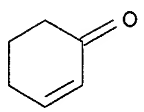
tetrahydroquinolines, such as (2R,4R)-2-methyl-4-bis(methoxycarbonyl)methyltetrahydroquinoline.

ED Entered STN: 04 Mar 2003

IT **930-68-7**, 2-Cyclohexen-1-one **5166-53-0**
RL: RCT (Reactant); **RACT (Reactant or reagent)**
(enantioselective Michael addition of malonates to acyclic α,β-unsatd. enones with imidazolidine catalyst)

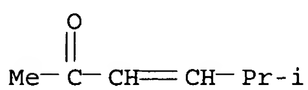
RN 930-68-7 HCAPLUS

CN 2-Cyclohexen-1-one (6CI, 8CI, 9CI) (CA INDEX NAME)



RN 5166-53-0 HCAPLUS

CN 3-Hexen-2-one, 5-methyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

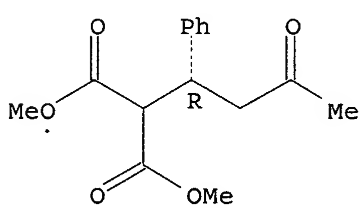


IT **109012-81-9P 196399-49-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(enantioselective Michael addition of malonates to acyclic α,β-unsatd. enones with imidazolidine catalyst)

RN 109012-81-9 HCAPLUS

CN Propanedioic acid, [(1R)-3-oxo-1-phenylbutyl]-, dimethyl ester (9CI) (CA INDEX NAME)

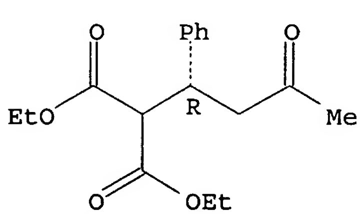
Absolute stereochemistry.



RN 196399-49-2 HCAPLUS

CN Propanedioic acid, [(1R)-3-oxo-1-phenylbutyl]-, diethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

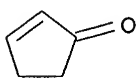


CC 23-17 (Aliphatic Compounds)
IT **Asymmetric synthesis and induction**
(enantioselective Michael addition of malonates to acyclic α,β-unsatd. enones with imidazolidine catalyst)
IT **Michael reaction**
Michael reaction catalysts
(stereoselective; enantioselective Michael addition of malonates to acyclic α,β-unsatd. enones with imidazolidine catalyst)
IT 105-53-3, Diethyl malonate 108-59-8, Dimethyl malonate 122-57-6, Benzylideneacetone 623-15-4 874-83-9 **930-68-7**, 2-Cyclohexen-1-one 1669-44-9, 3-Octen-2-one 1797-75-7 3152-68-9 3160-32-5 3160-35-8 3160-40-5 3490-37-7 4188-88-9 **5166-53-0** 5432-53-1 13195-64-7 15014-25-2, Dibenzyl malonate 20766-40-9 32864-38-3 42998-51-6 52267-39-7 61453-86-9 75032-63-2 89393-74-8
RL: RCT (Reactant); **RACT (Reactant or reagent)**
(enantioselective Michael addition of malonates to acyclic α,β-unsatd. enones with imidazolidine catalyst)
IT **109012-81-9P** 164931-75-3P **196399-49-2P** 541508-71-8P 541508-72-9P 541508-73-0P 541508-74-1P 541508-75-2P 541508-76-3P 541508-77-4P 541508-78-5P 541508-79-6P 541508-80-9P 541508-81-0P 541508-82-1P 541508-83-2P 541508-84-3P 541508-85-4P 541508-86-5P 541508-87-6P 541508-88-7P 541508-89-8P 541508-90-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(enantioselective Michael addition of malonates to acyclic α,β-unsatd. enones with imidazolidine catalyst)
REFERENCE COUNT: 57 THERE ARE 57 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

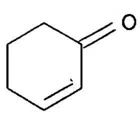
L93 ANSWER 9 OF 34 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2003:110333 HCAPLUS
DOCUMENT NUMBER: 138:287306
TITLE: Catalysis of the Michael Addition Reaction by Late Transition Metal Complexes of BINOL-Derived Salens
AUTHOR(S): Annamalai, Venkatachalam; DiMauro, Erin F.; Carroll, Patrick J.; Kozlowski, Marisa C.
CORPORATE SOURCE: Department of Chemistry, Roy and Diana Vagelos Laboratories, University of Pennsylvania, Philadelphia, PA, 19104-6323, USA
SOURCE: Journal of Organic Chemistry (**2003**), 68(5), 1973-1981
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 138:287306
AB Salen metal complexes incorporating two chiral BINOL moieties have been synthesized and characterized by X-ray crystallog. The X-ray structures show that this new class of Ni-BINOL-salen catalysts contains an unoccupied apical site for potential coordination of an electrophile and naphthoxides that are independent from the Lewis acid center. These characteristics allow independent alteration of the Lewis acidic and Bronsted basic sites. These unique complexes have been shown to catalyze the Michael reaction of dibenzyl malonate and cyclohexenone with good selectivity (up to 90% ee) and moderate yield (up to 79% yield). These catalysts

are also effective in the Michael reaction between other enones and malonates. Kinetic data show that the reaction is first order in the Ni·Cs-BINOL-salen catalyst. Further expts. probed the reactivity of the individual Lewis acid and Bronsted base components of the catalyst and established that both moieties are essential for asym. catalysis. All told, the data support a bifunctional activation pathway in which the apical Ni site of the Ni·Cs-BINOL-salen activates the enone and the naphthoxide base activates the malonate.

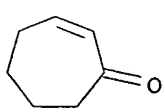
ED Entered STN: 13 Feb 2003
IT **930-30-3**, 2-Cyclopentenone **930-68-7**, 2-Cyclohexenone **1121-66-0**, 2-Cycloheptenone
RL: RCT (Reactant); RACT (Reactant or reagent)
(catalysis of the Michael addition reaction by late transition metal complexes of BINOL-derived salens)
RN 930-30-3 HCAPLUS
CN 2-Cyclopenten-1-one (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



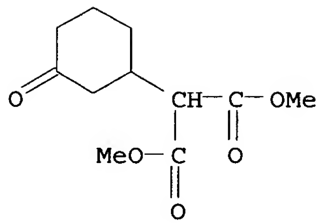
RN 930-68-7 HCAPLUS
CN 2-Cyclohexen-1-one (6CI, 8CI, 9CI) (CA INDEX NAME)



RN 1121-66-0 HCAPLUS
CN 2-Cyclohepten-1-one (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



IT **33646-18-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(catalysis of the Michael addition reaction by late transition metal complexes of BINOL-derived salens)
RN 33646-18-3 HCAPLUS
CN Propanedioic acid, (3-oxocyclohexyl)-, dimethyl ester (9CI) (CA INDEX NAME)



IT 349140-08-5P 349149-15-1P
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and crystal structure of nickel BINOL-derived salen-type catalysts for Michael addition reaction)

RN 349140-08-5 HCAPLUS

CN Nickel, [[(1S,1''S)-3,3''-[1,2-ethanediylbis[(nitrilo-κN)methylidyne]]bis[[1,1'-binaphthalene]-2,2'-diolato-κO2]](2-)]-, (SP-4-2)- (9CI) (CA INDEX NAME)

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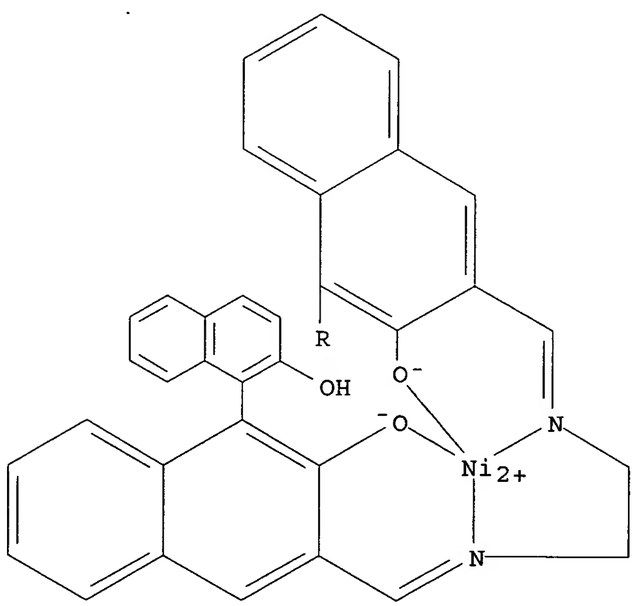
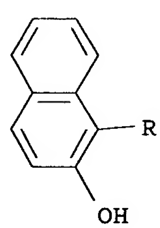
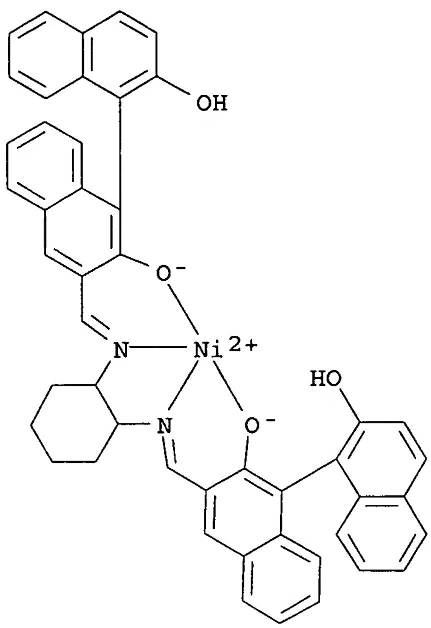


PAGE 2-A

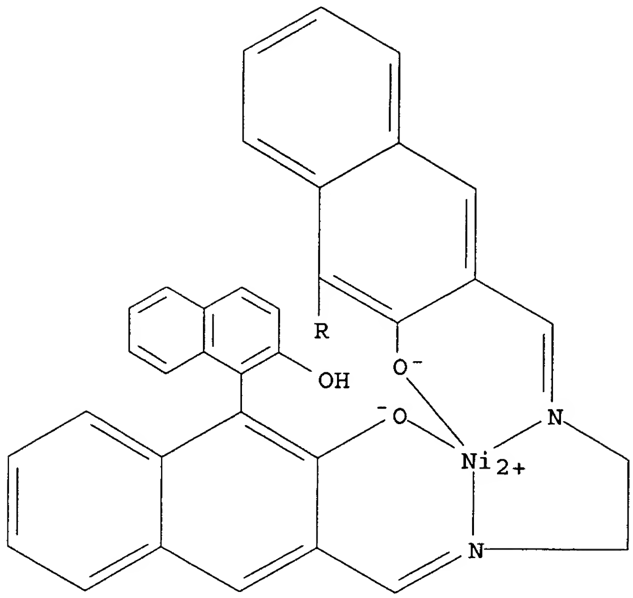


RN 349149-15-1 HCAPLUS
CN Nickel, [[(1S,1''S)-3,3''-[(1R,2R)-1,2-cyclohexanediylbis[(nitrilo-κN)methylidyne]]bis[[1,1'-binaphthalene]-2,2'-diolato-κO2]](2-)]-, (SP-4-2)- (9CI) (CA INDEX NAME)

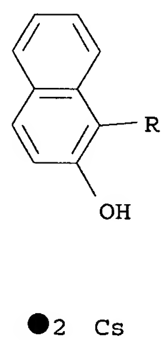


IT **349140-17-6P 349140-18-7P 349149-18-4P 504394-83-6P 504409-95-4P 504410-02-0P 504410-04-2P**
RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(preparation of nickel BINOL-derived salen-type catalysts for Michael addition reaction)
RN 349140-17-6 HCAPLUS
CN Nickelate(2-), [[(1S,1''S)-3,3''-[1,2-ethanediylbis[(nitrilo-κN)methylidyne]]bis[[1,1'-binaphthalene]-2,2'-diolato-κO2]](4-)]-, dicesium, (SP-4-2)- (9CI) (CA INDEX NAME)

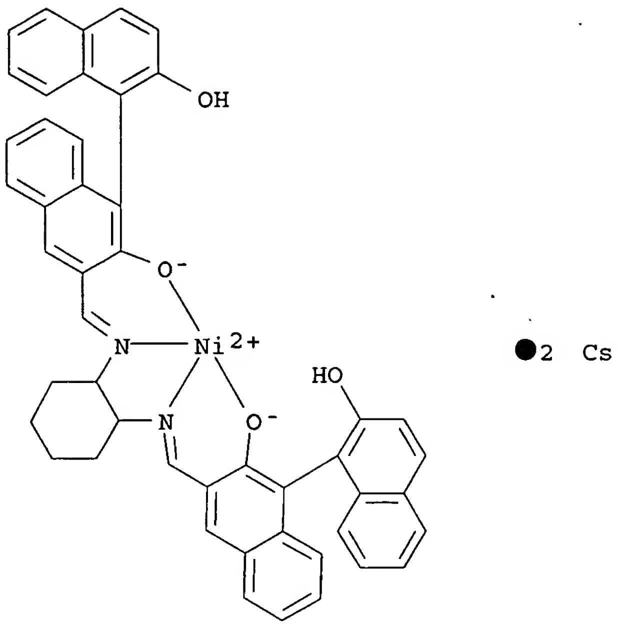
PAGE 1-A



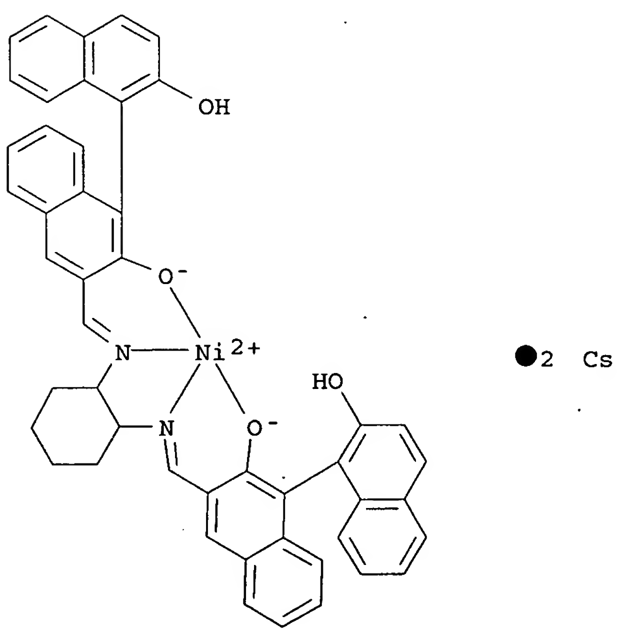
PAGE 2-A



RN 349140-18-7 HCAPLUS
CN Nickelate(2-), [[(1S,1''S)-3,3''-[(1S,2S)-1,2-cyclohexanediylbis[(nitrilo-κN)methylidyne]]bis[[1,1'-binaphthalene]-2,2'-diolato-κO2]](4-)]-, dicesium, (SP-4-2)-(9CI) (CA INDEX NAME)



RN 349149-18-4 HCAPLUS
CN Nickelate(2-), [[(1S,1''S)-3,3''-[(1R,2R)-1,2-cyclohexanediylbis[(nitrilo-κN)methylidyne]]bis[[1,1'-binaphthalene]-2,2'-diolato-κO2]](4-)]-, dicesium, (SP-4-2)- (9CI) (CA INDEX NAME)



RN 504394-83-6 HCAPLUS
CN Nickel, [[(1S,1''S)-3,3''-[1,2-ethanediylbis[(nitrilo-κN)methylidyne]]bis[2'-methoxy[1,1'-binaphthalen]-2-olato-κO]](2-)]-, (SP-4-2)- (9CI) (CA INDEX NAME)

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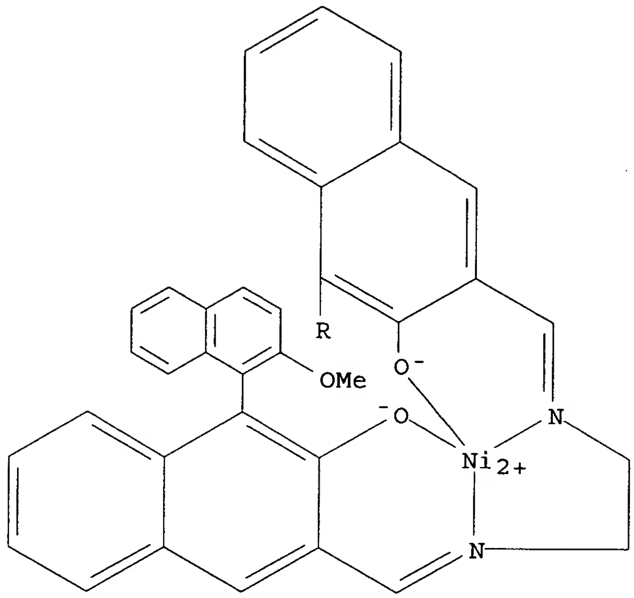

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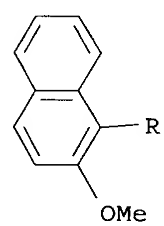
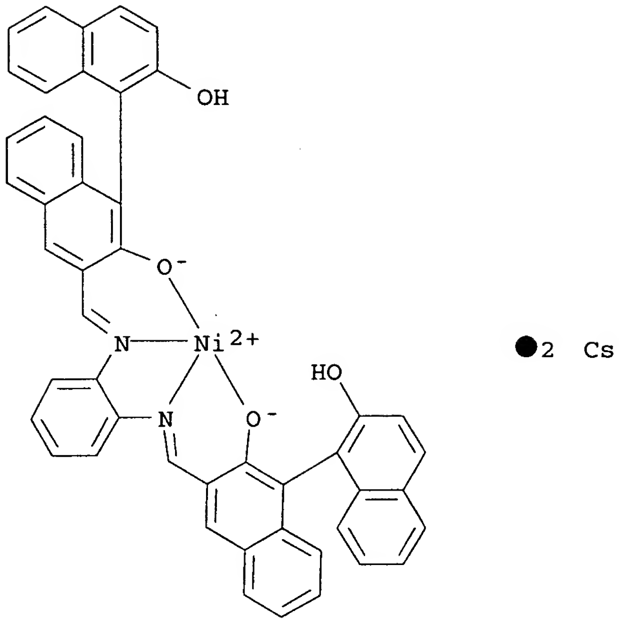
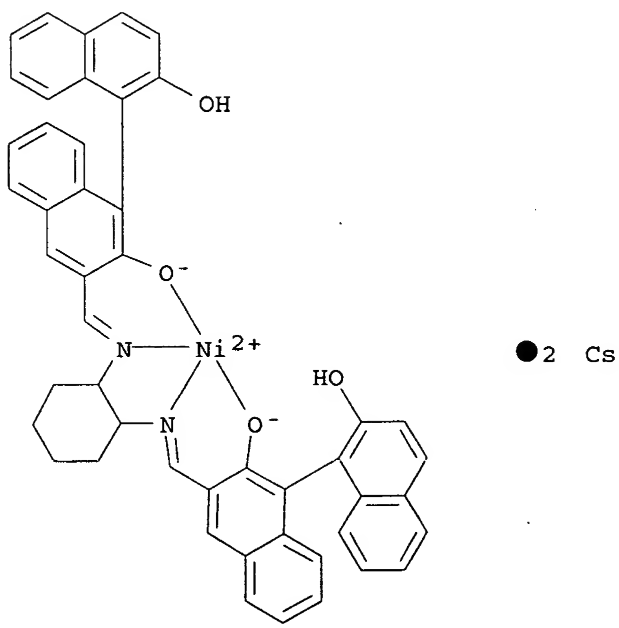


RN 504409-95-4 HCAPLUS
CN Nickel, [[(1S,1''S)-3,3''-[1,2-phenylenebis[(nitrilo-κN)methylidyne]]bis[[1,1'-binaphthalene]-2,2'-diolato-κO2]](2-)]-, dicesium salt, (SP-4-2)- (9CI) (CA INDEX NAME)



RN 504410-02-0 HCAPLUS
CN Nickel, [[(1S,1''S)-3,3''-[(1R,2S)-1,2-cyclohexanediylbis[(nitrilo-κN)methylidyne]]bis[[1,1'-binaphthalene]-2,2'-diolato-κO2]](2-)]-, dicesium salt, (SP-4-4)- (9CI) (CA INDEX NAME)



RN 504410-04-2 HCAPLUS
CN Nickel, [[(1S,1''S)-3,3''-[[(1R,2R)-1,2-diphenyl-1,2-ethanediyl]bis[(nitrilo-κN)methylidyne]]bis[[1,1'-binaphthalene]-2,2'-diolato-κO2]](2-)]-, dicesium salt, (SP-4-2)- (9CI) (CA INDEX NAME)

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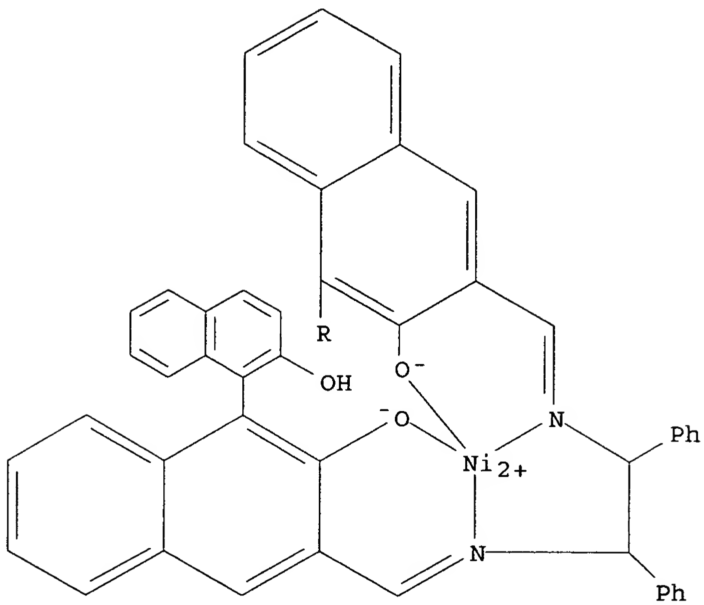

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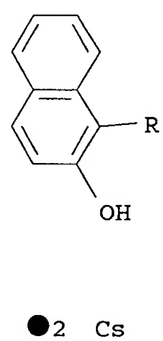
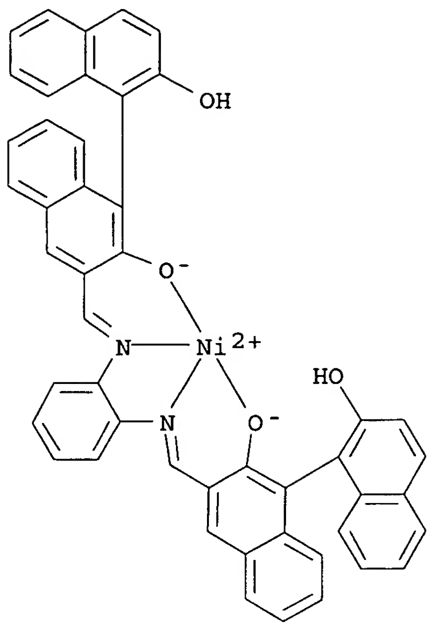


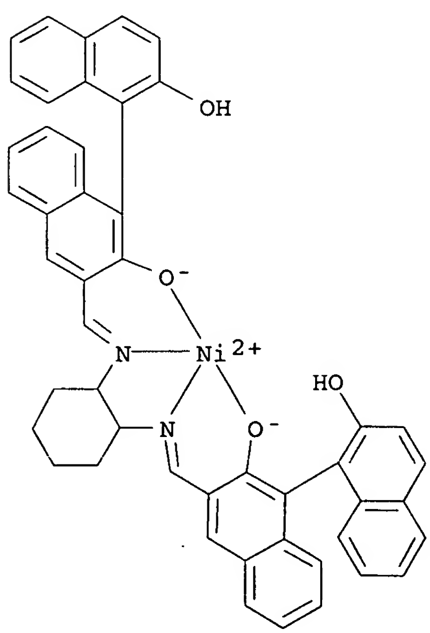
IT 349140-12-1P 349140-14-3P 349140-16-5P
349149-17-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of nickel BINOL-derived salen-type catalysts for Michael addition reaction)

RN 349140-12-1 HCAPLUS

CN Nickel, [[(1S,1''S)-3,3''-[1,2-phenylenebis[(nitrilo-κN)methylidyne]]bis[[1,1'-binaphthalene]-2,2'-diolato-κO2]](2-)]-, (SP-4-2)- (9CI) (CA INDEX NAME)



RN 349140-14-3 HCAPLUS
CN Nickel, [[(1S,1''S)-3,3''-[(1S,2S)-1,2-cyclohexanediylbis[(nitrilo-κN)methylidyne]]bis[[1,1'-binaphthalene]-2,2'-diolato-κO2]](2-)]-, (SP-4-2)- (9CI) (CA INDEX NAME)



RN 349140-16-5 HCAPLUS
CN Nickel, [[(1S,1''S)-3,3''-[[(1R,2R)-1,2-diphenyl-1,2-ethanediyl]bis[(nitrilo-κN)methylidyne]]bis[[1,1'-binaphthalene]-2,2'-diolato-κO2]](2-)]-, (SP-4-2)- (9CI) (CA INDEX NAME)

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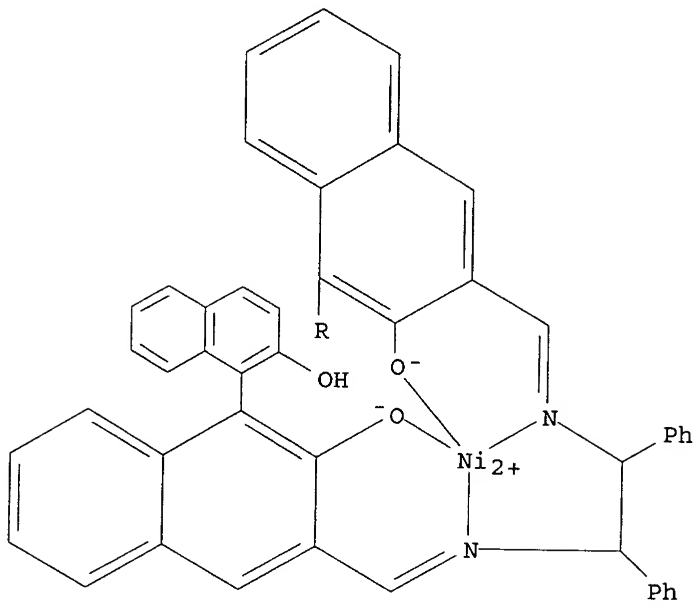

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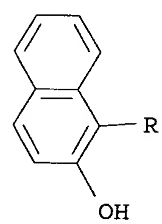
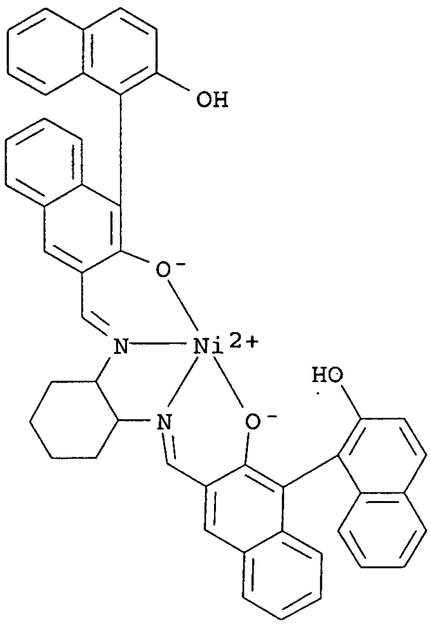
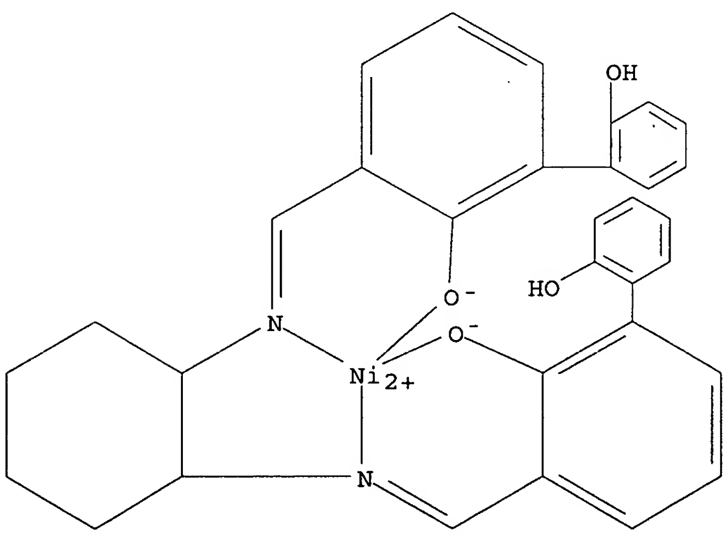


RN 349149-17-3 HCAPLUS
CN Nickel, [[(1S,1''S)-3,3''-[(1R,2S)-1,2-cyclohexanediylbis[(nitrilo-κN)methylidyne]]bis[[1,1'-binaphthalene]-2,2'-diolato-κO2]](2-)]-, (SP-4-4)- (9CI) (CA INDEX NAME)



IT 504394-80-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of nickel BINOL-derived salen-type catalysts for Michael addition reaction)
RN 504394-80-3 HCAPLUS
CN Nickel, [[3,3''-[(1R,2R)-1,2-cyclohexanediylbis[(nitrilo-κN)methylidyne]]bis[[1,1'-biphenyl]-2,2'-diolato-κO2]](2-)]-, (SP-4-2)- (9CI) (CA INDEX NAME)



CC 24-5 (Alicyclic Compounds)
Section cross-reference(s): 25, 78
IT **Michael reaction**
Michael reaction catalysts

(stereoselective; catalysis of the Michael addition reaction by late transition metal complexes of BINOL-derived salens)

IT 108-59-8, Dimethyl malonate 614-47-1, trans-Chalcone **930-30-3**, 2-Cyclopentenone **930-68-7**, 2-Cyclohexenone **1121-66-0**, 2-Cycloheptenone 5153-67-3, trans-β-Nitrostyrene 15014-25-2, Dibenzyl malonate
RL: RCT (Reactant); RACT (Reactant or reagent)
(catalysis of the Michael addition reaction by late transition metal complexes of BINOL-derived salens)

IT **33646-18-3P** 55790-16-4P 67488-98-6P 164931-75-3P 181712-81-2P 504394-81-4P 504394-82-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(catalysis of the Michael addition reaction by late transition metal complexes of BINOL-derived salens)

IT **349140-08-5P 349149-15-1P**
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and crystal structure of nickel BINOL-derived salen-type catalysts for Michael addition reaction)

IT **349140-17-6P 349140-18-7P 349149-18-4P 504394-83-6P 504409-95-4P 504410-02-0P 504410-04-2P**
RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(preparation of nickel BINOL-derived salen-type catalysts for Michael addition reaction)

IT 156660-22-9P, 2,2'-Dihydroxy-1,1'-biphenyl-3-carboxaldehyde 209908-74-7P **349140-12-1P 349140-14-3P 349140-16-5P** 349149-09-3P 349149-10-6P 349149-11-7P 349149-12-8P 349149-13-9P 349149-14-0P **349149-17-3P** 504394-79-0P 504407-87-8P 504407-88-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of nickel BINOL-derived salen-type catalysts for Michael addition reaction)

IT **504394-80-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of nickel BINOL-derived salen-type catalysts for Michael addition reaction)

REFERENCE COUNT: 44 THERE ARE 44 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L93 ANSWER 10 OF 34 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2003:67244 HCAPLUS
DOCUMENT NUMBER: 139:6420
TITLE: Novel heterobimetallic catalysts for asymmetric Michael reactions
AUTHOR(S): Velmathi, S.; Swarnalakshmi, S.; Narasimhan, S.
CORPORATE SOURCE: T.R. Govindachari Centre for Natural Products, SPIC Science Foundation, Chennai, 600 032, India
SOURCE: Tetrahedron: Asymmetry (**2003**), 14(1), 113-117
CODEN: TASYE3; ISSN: 0957-4166
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 139:6420

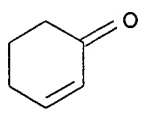
AB The newly developed chiral catalysts based on organoborane and organoaluminum complexes show opposite enantioselectivity in Michael addition reactions of cyclic enones and malonates resulting in the production of both enantiomers of products in good chemical yield and enantiomeric excess. 27Al NMR studies showed the formation of different types of complexes for these catalysts and the enantioselectivity was found to be dependent on the nature of the aluminum complex formed. Scope of the reaction was extended to other Michael donors such as nitro alkanes and thiols.

ED Entered STN: 29 Jan 2003

IT **930-68-7**, 2-Cyclohexenone
RL: RCT (Reactant); **RACT (Reactant or reagent)**
(asym. Michael addition reactions of cyclic enones and malonates in presence of organoaluminum and organoborane complex catalysts)

RN 930-68-7 HCAPLUS

CN 2-Cyclohexen-1-one (6CI, 8CI, 9CI) (CA INDEX NAME)

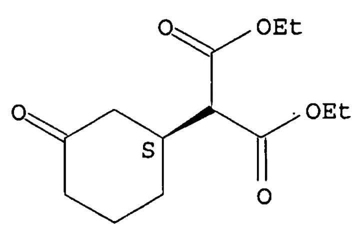


IT **151600-50-9P 164931-78-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(asym. Michael addition reactions of cyclic enones and malonates in presence of organoaluminum and organoborane complex catalysts)

RN 151600-50-9 HCAPLUS

CN Propanedioic acid, [(1S)-3-oxocyclohexyl]-, diethyl ester (9CI) (CA INDEX NAME)

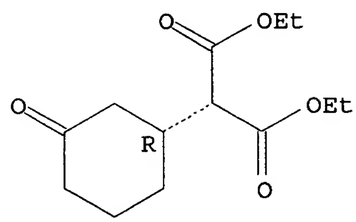
Absolute stereochemistry. Rotation (-).



RN 164931-78-6 HCAPLUS

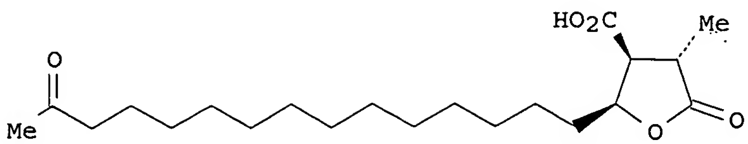
CN Propanedioic acid, [(1R)-3-oxocyclohexyl]-, diethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



CC 21-2 (General Organic Chemistry)
IT **Asymmetric synthesis and induction**
(of cyclohexane malonates and acyclic α,β-unsatd. enones and enols in presence of organoaluminum and organoborane complexes)
IT **Michael reaction**
(stereoselective; of cyclohexanone with di-Et malonate and malonic esters, nitro alkanes, and thiols in presence of organoaluminum and organoborane complex **catalysts**)
IT **Michael reaction catalysts**
(stereoselective; organoaluminum and organoborane complex catalysts for asym. Michael addition of cyclohexanone with di-Et malonate and malonic esters, nitro alkanes, and thiols)
IT 105-53-3, Diethyl malonate **930-68-7**, 2-Cyclohexenone
RL: RCT (Reactant); **RACT (Reactant or reagent)**
(asym. Michael addition reactions of cyclic enones and malonates in presence of organoaluminum and organoborane complex catalysts)
IT **151600-50-9P 164931-78-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(asym. Michael addition reactions of cyclic enones and malonates in presence of organoaluminum and organoborane complex catalysts)
REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L93 ANSWER 11 OF 34 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2003:4446 HCAPLUS
DOCUMENT NUMBER: 138:237913
TITLE: Synthesis of (±)-nephromopsinic, (-)-phaseolinic, and (-)-dihydropertusaric acids
AUTHOR(S): Brecht-Forster, Andrea; Fitremann, Juliette; Renaud, Philippe
CORPORATE SOURCE: Universite de Fribourg, Departement de Chimie, Fribourg, CH-1700, Switz.
SOURCE: Helvetica Chimica Acta (**2002**), 85(11), 3965-3974
CODEN: HCACAV; ISSN: 0018-019X
PUBLISHER: Verlag Helvetica Chimica Acta
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 138:237913
GI



I

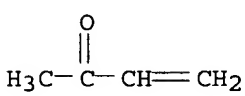
AB The formal syntheses of (±)-nephromopsinic acid, (-)-phaseolinic acid, and the first total synthesis of (-)-dihydropertusaric acid (I) from (±)- and (-)-7-oxabicyclo[2.2.1]hept-5-en-2-one are described. These syntheses take advantage of a previously reported radical rearrangement (1,2-acyl migration). A remarkable iodide-mediated cleavage of a bicyclic system, followed by the introduction of the γ-chains via a mixed Kolbe electrolysis, are the key steps of these syntheses. This approach is general and could be applied for the preparation of all kinds of paraconic acids with excellent control of the stereochem.

ED Entered STN: 03 Jan 2003

IT **78-94-4**, Methyl vinyl ketone
RL: RCT (Reactant); **RACT (Reactant or reagent)**
(preparation of (-)-dihydropertusaric acid and formal synthesis of (±)-nephromopsinic, and (-)-phaseolinic acids)

RN 78-94-4 HCAPLUS

CN 3-Buten-2-one (8CI, 9CI) (CA INDEX NAME)

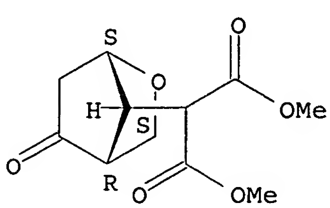


IT **152469-10-8P 501666-59-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of (-)-dihydropertusaric acid and formal synthesis of (±)-nephromopsinic, and (-)-phaseolinic acids)

RN 152469-10-8 HCAPLUS

CN Propanedioic acid, [(1R,4S,7R)-5-oxo-2-oxabicyclo[2.2.1]hept-7-yl]-, dimethyl ester, rel- (9CI) (CA INDEX NAME)

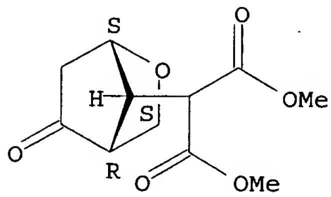
Relative stereochemistry.



RN 501666-59-7 HCAPLUS

CN Propanedioic acid, [(1S,4R,7S)-5-oxo-2-oxabicyclo[2.2.1]hept-7-yl]-, dimethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



CC 26-6 (Biomolecules and Their Synthetic Analogs)
Section cross-reference(s): 72

IT **Asymmetric synthesis and induction**
(of (-)-dihydropertusaric acid)

IT **78-94-4**, Methyl vinyl ketone 109-52-4D, n-Pentanoic acid, derivs. 112-43-6, Undec-10-en-1-ol 127-19-5D, N,N-Dimethylacetamide, derivs. 638-53-9, Tridecanoic acid 72041-43-1 94482-75-4 95530-78-2, 7-Oxabicyclo[2.2.1]hept-5-en-2-one 501666-57-5
RL: RCT (Reactant); **RACT (Reactant or reagent)**
(preparation of (-)-dihydropertusaric acid and formal synthesis of (±)-nephromopsinic, and (-)-phaseolinic acids)

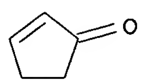
IT 39115-08-7P **152469-10-8P** 208587-00-2P 214531-60-9P 214531-61-0P 214531-62-1P 214531-63-2P 214531-64-3P 501666-52-0P 501666-53-1P 501666-54-2P 501666-55-3P 501666-56-4P 501666-58-6P **501666-59-7P** 501666-60-0P 501666-61-1P 501669-34-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of (-)-dihydropertusaric acid and formal synthesis of (±)-nephromopsinic, and (-)-phaseolinic acids)

REFERENCE COUNT: 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

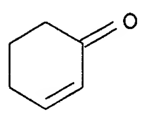
L93 ANSWER 12 OF 34 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2003:3194 HCAPLUS
DOCUMENT NUMBER: 138:353501
TITLE: Enantioselective Michael addition and Henry reaction catalyzed by a new heterobimetallic aluminum-lithium complex derived from (+)-2,3-O-isopropylidine threitol
AUTHOR(S): Rajasekhar, Ch V.; Maheswaran, H.
CORPORATE SOURCE: Indian Institute of Chemical Technology, Hyderabad, 500 007, India
SOURCE: Indian Journal of Chemistry, Section A: Inorganic, Bio-inorganic, Physical, Theoretical & Analytical Chemistry (**2002**), 41A(12), 2503-2506
CODEN: ICACEC; ISSN: 0376-4710
PUBLISHER: National Institute of Science Communication
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 138:353501

AB A heterobimetallic catalyst obtained by the reaction of $LiAlH_4$ with (+)-2,3-O-isopropylidine threitol promotes asym. Michael reaction (between malonic esters, and thiophenols to cyclic enones) as well as Henry reaction (between aliphatic and aromatic aldehydes and nitromethane) with excellent yields albeit low enantiomeric excesses.

ED Entered STN: 03 Jan 2003
IT **930-30-3**, 2-Cyclopentenone **930-68-7**,
2-Cyclohexenone
RL: RCT (Reactant); **RACT (Reactant or reagent)**
(enantioselective Michael addition of cycloenones with malonates or thiophenols and Henry reaction of aldehydes with nitromethane catalyzed by heterobimetallic aluminum-lithium complex derived from (+)-2,3-O-isopropylidine threitol)
RN 930-30-3 HCAPLUS
CN 2-Cyclopenten-1-one (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

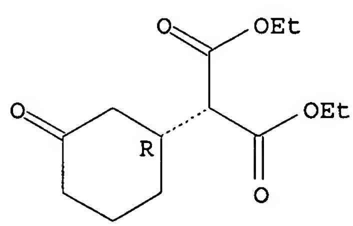


RN 930-68-7 HCAPLUS
CN 2-Cyclohexen-1-one (6CI, 8CI, 9CI) (CA INDEX NAME)



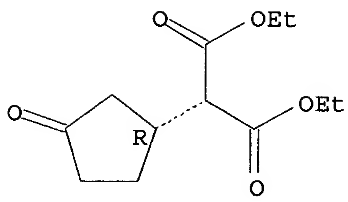
IT **164931-78-6P 194095-90-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(enantioselective Michael addition of cycloenones with malonates or thiophenols and Henry reaction of aldehydes with nitromethane catalyzed by heterobimetallic aluminum-lithium complex derived from (+)-2,3-O-isopropylidine threitol)
RN 164931-78-6 HCAPLUS
CN Propanedioic acid, [(1R)-3-oxocyclohexyl]-, diethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



RN 194095-90-4 HCAPLUS
CN Propanedioic acid, [(1R)-3-oxocyclopentyl]-, diethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



CC 21-2 (General Organic Chemistry)
Section cross-reference(s): 67

IT **Alkylation**
(Henry, nitroaldol; enantioselective **Michael** addition of cycloenones with malonates or thiophenols and Henry reaction of aldehydes with nitromethane catalyzed by heterobimetallic aluminum-lithium complex derived from (+)-2,3-O-isopropylidine threitol)

IT **Asymmetric synthesis and induction**
(enantioselective Michael addition of cycloenones with malonates or thiophenols and Henry reaction of aldehydes with nitromethane catalyzed by heterobimetallic aluminum-lithium complex derived from (+)-2,3-O-isopropylidine threitol)

IT **Michael reaction**
(stereoselective; enantioselective Michael addition of cycloenones with malonates or thiophenols and Henry reaction of aldehydes with nitromethane catalyzed by heterobimetallic aluminum-lithium complex derived from (+)-2,3-O-isopropylidine threitol)

IT 100-52-7, Benzaldehyde, reactions 104-53-0, 3-Phenylpropanal 104-87-0, p-Methylbenzaldehyde 105-53-3, Ethyl malonate 106-54-7, p-Chlorothiophenol 123-38-6, Propanal, reactions **930-30-3**, 2-Cyclopentenone **930-68-7**, 2-Cyclohexenone
RL: RCT (Reactant); **RACT (Reactant or reagent)**
(enantioselective Michael addition of cycloenones with malonates or thiophenols and Henry reaction of aldehydes with nitromethane catalyzed by heterobimetallic aluminum-lithium complex derived from (+)-2,3-O-isopropylidine threitol)

IT 64924-10-3P 141434-97-1P 149495-00-1P **164931-78-6P** **194095-90-4P** 259811-41-1P 518328-48-8P 518328-49-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(enantioselective Michael addition of cycloenones with malonates or thiophenols and Henry reaction of aldehydes with nitromethane catalyzed by heterobimetallic aluminum-lithium complex derived from (+)-2,3-O-isopropylidine threitol)

REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L93 ANSWER 13 OF 34 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2002:863839 HCAPLUS
DOCUMENT NUMBER: 139:85391
TITLE: Product subclass 16: silyl enol ethers
AUTHOR(S): Kobayashi, S.; Manabe, K.; Ishitani, H.; Matsuo, J.-I.
CORPORATE SOURCE: Graduate School of Pharmaceutical Sciences, The University of Tokyo, Hongo, Bunkyo-ku, Tokyo, 113-0033, Japan
SOURCE: Science of Synthesis (2002), 4,

317-369
CODEN: SSCYJ9
PUBLISHER: Georg Thieme Verlag
DOCUMENT TYPE: Journal; **General Review**
LANGUAGE: English

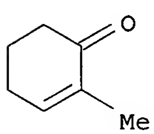
AB A review of preparation and reactions of silyl enol ethers. Covered reactions include addition, alkylation, Mukaiyama reaction, aldol condensation, cycloaddn., Mannich reaction, Diels-Alder reaction, amination, Ireland-Claisen rearrangement, hydroxylation, and silylation.

ED Entered STN: 14 Nov 2002

IT **1121-18-2**
RL: RCT (Reactant); **RACT (Reactant or reagent)**
(addition of furan and bis(trimethylsilane) amine; preparation of silyl enol ethers via reductive silylation of α,β-unsatd. carbonyl compound)

RN 1121-18-2 HCAPLUS

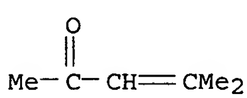
CN 2-Cyclohexen-1-one, 2-methyl- (7CI, 8CI, 9CI) (CA INDEX NAME)



IT **141-79-7**
RL: RCT (Reactant); **RACT (Reactant or reagent)**
(preparation of silyl enol ethers via hydrosilylation of α,β-unsatd. carbonyl compound)

RN 141-79-7 HCAPLUS

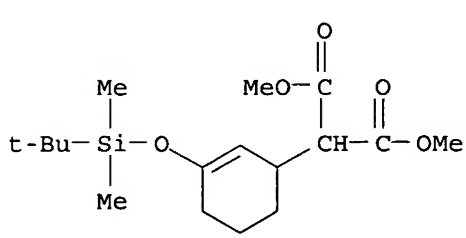
CN 3-Penten-2-one, 4-methyl- (8CI, 9CI) (CA INDEX NAME)



IT **152094-29-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of silyl enol ethers via reductive silylation of α,β-unsatd. carbonyl compound)

RN 152094-29-6 HCAPLUS

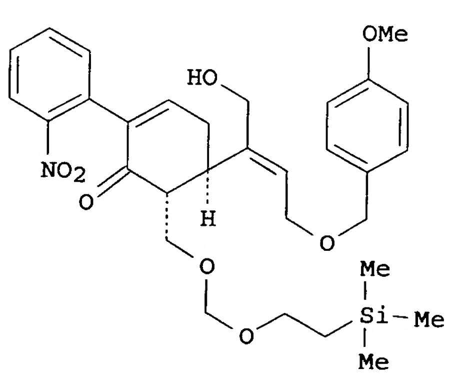
CN Propanedioic acid, [3-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-2-cyclohexen-1-yl]-, dimethyl ester (9CI) (CA INDEX NAME)



CC 29-0 (Organometallic and Organometalloidal Compounds)

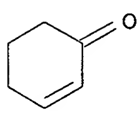
IT **Asymmetric synthesis and induction**
(asym. aldol reaction of chiral silyl enol ether with achiral benzaldehyde)
IT **1121-18-2**
RL: RCT (Reactant); **RACT (Reactant or reagent)**
(addition of furan and bis(trimethylsilane) amine; preparation of silyl enol ethers via reductive silylation of α,β-unsatd. carbonyl compound)
IT **141-79-7** 18707-60-3
RL: RCT (Reactant); **RACT (Reactant or reagent)**
(preparation of silyl enol ethers via hydrosilylation of α,β-unsatd. carbonyl compound)
IT 62790-93-6P 78905-92-7P 105229-94-5P 106251-78-9P 108612-95-9P 138593-34-7P 146273-75-8P **152094-29-6P** 160915-46-8P 177658-19-4DP, polymer-bound 441011-27-4P 556813-33-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of silyl enol ethers via reductive silylation of α,β-unsatd. carbonyl compound)
REFERENCE COUNT: 418 THERE ARE 418 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L93 ANSWER 14 OF 34 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2002:863063 HCAPLUS
DOCUMENT NUMBER: 138:89950
TITLE: Enantioselective Total Synthesis of (-)-Strychnine Using the Catalytic Asymmetric Michael Reaction and Tandem Cyclization
AUTHOR(S): Ohshima, Takashi; Xu, Youjun; Takita, Ryo; Shimizu, Satoshi; Zhong, Dafang; Shibasaki, Masakatsu
CORPORATE SOURCE: Graduate School of Pharmaceutical Sciences, University of Tokyo, Tokyo, 113-0033, Japan
SOURCE: Journal of the American Chemical Society (**2002**), 124(49), 14546-14547
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 138:89950
GI



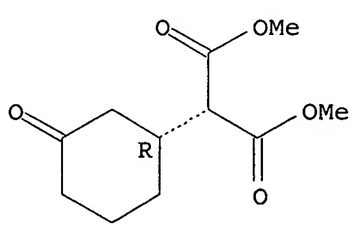
I

AB The enantioselective total synthesis of (-)-strychnine was accomplished through the use of the highly practical catalytic asym. Michael reaction of 2-cyclohexen-1-one with di-Me malonate (0.1 mol % of (R)-ALB, more than kilogram scale, without chromatog., 91% yield and >99% ee) as well as a tandem cyclization of (nitrophenyl)propenylcyclohexenone I that simultaneously constructed B- and D-rings (>77% yield). Moreover, newly developed reaction conditions for thionium ion cyclization, NaBH3CN reduction of the imine moiety in the presence of Lewis acid to prevent ring opening reaction, and chemoselective reduction of the thioether (desulfurization) in the presence of exocyclic olefin were pivotal to complete the synthesis. The described chemical paves the way for the synthesis of more advanced Strychnos alkaloids.
ED Entered STN: 14 Nov 2002
IT **930-68-7**, 2-Cyclohexen-1-one
RL: RCT (Reactant); **RACT (Reactant or reagent)**
(asym. total synthesis of (-)-strychnine via catalytic asym. Michael reaction and tandem cyclization)
RN 930-68-7 HCAPLUS
CN 2-Cyclohexen-1-one (6CI, 8CI, 9CI) (CA INDEX NAME)



IT **164931-77-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(asym. total synthesis of (-)-strychnine via catalytic asym. Michael reaction and tandem cyclization)
RN 164931-77-5 HCAPLUS
CN Propanedioic acid, [(1R)-3-oxocyclohexyl]-, dimethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



CC 31-4 (Alkaloids)
IT **Asymmetric synthesis and induction**
(asym. total synthesis of (-)-strychnine via catalytic asym. Michael reaction and tandem cyclization)
IT **Michael reaction**
Michael reaction catalysts
(stereoselective; asym. total synthesis of (-)-strychnine via catalytic asym. Michael reaction and tandem cyclization)
IT 108-59-8, Dimethyl malonate 126-39-6, 2-Ethyl-2-methyl-1,3-

dioxolane 141-82-2, Malonic acid, reactions **930-68-7**, 2-Cyclohexen-1-one 13154-24-0 17341-93-4, 2,2,2-Trichloroethoxycarbonyl chloride 76513-69-4 80522-42-5, Triisopropylsilyl triflate 122807-21-0 191731-32-5 482351-25-7
RL: RCT (Reactant); **RACT (Reactant or reagent)**
(asym. total synthesis of (-)-strychnine via catalytic asym. Michael reaction and tandem cyclization)

IT 509-40-0P 71366-23-9P **164931-77-5P** 482351-05-3P
482351-06-4P 482351-07-5P 482351-08-6P 482351-09-7P
482351-10-0P 482351-11-1P 482351-12-2P 482351-13-3P
482351-14-4P 482351-15-5P 482351-16-6P 482351-18-8P
482351-19-9P 482351-20-2P 482351-21-3P 482351-22-4P
482351-26-8P 482351-27-9P 482351-28-0P 482351-29-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(asym. total synthesis of (-)-strychnine via catalytic asym. Michael reaction and tandem cyclization)

REFERENCE COUNT: 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

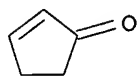
L93 ANSWER 15 OF 34 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2002:456602 HCAPLUS
DOCUMENT NUMBER: 138:4183
TITLE: Highly enantioselective catalytic Michael reaction of α-substituted malonates using La-linked-BINOL complex in the presence of HFIP (1,1,1,3,3,3-hexafluoroisopropanol)
AUTHOR(S): Takita, Ryo; Ohshima, Takashi; Shibasaki, Masakatsu
CORPORATE SOURCE: Graduate School of Pharmaceutical Sciences, The University of Tokyo, Tokyo, 113-0033, Japan
SOURCE: Tetrahedron Letters (**2002**), 43(26), 4661-4665
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 138:4183

AB A catalytic asym. Michael reaction of α-substituted malonates with broad generality was developed using the La-linked-BINOL complex. To enhance the reactivity of unreactive α-substituted malonates, the effects of concentration and additives were examined; 1.0 M was the best concentration and HFIP (1,1,1,3,3,3-hexafluoroisopropanol) accelerated the reaction efficiently. Under the optimized conditions, the catalytic asym. Michael reaction of a variety of α-substituted malonates proceeded successfully in high yield (up to 93%) and excellent enantiomeric excess (up to 99% ee). The addition of HFIP was also effective for the reaction of nonsubstituted malonates. In this case, 5 mol% of the La-linked-BINOL complex was sufficient for completion of the reaction in approx. 24 h. Moreover, several Michael adducts were readily converted to the bicyclic compds.

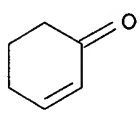
ED Entered STN: 18 Jun 2002

IT **930-30-3**, 2-Cyclopentenone **930-68-7**, 2-Cyclohexenone **1121-66-0**, 2-Cycloheptenone
RL: RCT (Reactant); **RACT (Reactant or reagent)**
(enantioselective Michael reaction of malonates with

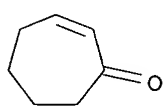
cycloalkenones using La-linked-BINOL complex
catalyst/hexafluoroisopropanol accelerator systems)
RN 930-30-3 HCAPLUS
CN 2-Cyclopenten-1-one (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



RN 930-68-7 HCAPLUS
CN 2-Cyclohexen-1-one (6CI, 8CI, 9CI) (CA INDEX NAME)

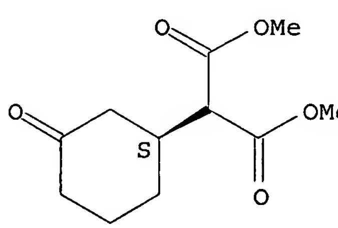


RN 1121-66-0 HCAPLUS
CN 2-Cyclohepten-1-one (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



IT **154194-50-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(enantioselective Michael reaction of malonates with
cycloalkenones using La-linked-BINOL complex
catalyst/hexafluoroisopropanol accelerator systems)
RN 154194-50-0 HCAPLUS
CN Propanedioic acid, [(1S)-3-oxocyclohexyl]-, dimethyl ester (9CI)
(CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



CC 21-2 (General Organic Chemistry)
IT **Asymmetric synthesis and induction**
(enantioselective Michael reaction of malonates with
cycloalkenones using La-linked-BINOL complex
catalyst/hexafluoroisopropanol accelerator systems)
IT **Michael reaction**
Michael reaction catalysts
(stereoselective; enantioselective Michael reaction of

malonates with cycloalkenones using La-linked-BINOL complex catalyst/hexafluoroisopropanol accelerator systems)

IT 108-59-8, Dimethyl malonate **930-30-3**, 2-Cyclopentenone **930-68-7**, 2-Cyclohexenone **1121-66-0**, 2-Cycloheptenone 15014-25-2, Dibenzyl malonate 173541-54-3 173979-06-1 476437-46-4 476437-50-0 476437-52-2 476437-54-4 476437-55-5

RL: RCT (Reactant); **RACT (Reactant or reagent)**
(enantioselective Michael reaction of malonates with cycloalkenones using La-linked-BINOL complex catalyst/hexafluoroisopropanol accelerator systems)

IT 154194-47-5P 154194-49-7P **154194-50-0P** 476437-56-6P 476437-58-8P 476437-59-9P 476437-61-3P 476437-65-7P 476437-67-9P 476437-71-5P

RL: SPN (Synthetic preparation); PREP (Preparation)
(enantioselective Michael reaction of malonates with cycloalkenones using La-linked-BINOL complex catalyst/hexafluoroisopropanol accelerator systems)

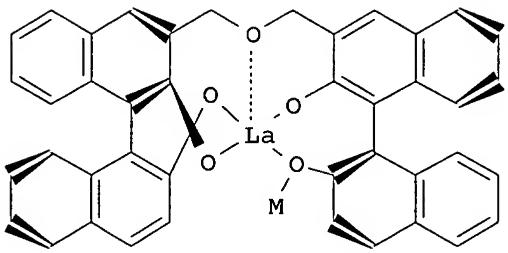
REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L93 ANSWER 16 OF 34 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2002:169599 HCAPLUS
DOCUMENT NUMBER: 136:240696
TITLE: Preparation of lanthanum-linked bis(BINOL) complexes as catalysts for asymmetric Michael addition reaction
INVENTOR(S): Shibazaki, Masakatsu; Oshima, Takashi; Matsunaga, Shigeki
PATENT ASSIGNEE(S): Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 11 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2002069076	A2	20020308	JP 2000-262411 <--	2000 0831
TW 552265	B	20030911	TW 2000-89118379 <--	2000 0905

PRIORITY APPLN. INFO.: JP 2000-262411 A 2000 0831 <--

OTHER SOURCE(S): CASREACT 136:240696
GI



I

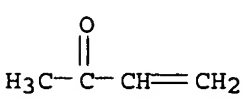
AB The bis[[(1R,1'R)-2,2'-dihydroxy-1,1'-binaphthyl-3-yl]methyl] ether-lanthanum complexes (I; M = H, monovalent metal atom) and an acid composition containing I are prepared These complexes I catalyze asym. Michael addition reaction of β-dicarbonyl compds. with cyclic or noncyclic enones. They are very stable even in air and can be stored for a long period of time and reused. Thus, 7.5 mL of 0.2M La(O-i-Pr)3/THF (1.5 mmol) was added to a solution of 1.01 g bis[[(1R,1'R)-2,2'-Dihydroxy-1,1'-binaphthyl-3-yl]methyl] ether (containing 7.4 weight/weight% Et2O and hexane) in 10 mL THF and stirred at room temperature for 5 h to give 1.13 g I (M = H). I (M = H) (45.1 mg) was added to 1.5 mL 1,2-dimethoxyethane at -78° in an acetone-dry ice bath and stirred for 5 min, followed by adding 58 μL 2-cyclohexen-1-one (0.60 mmol) and 150 μL dibenzyl malonate (0.60 mmol), and the resulting mixture was stirred at -78° in the acetone-dry ice bath and at 4° for 85 h after removing the bath to give 98% (R)-3-[bis(benzyloxycarbonyl)methyl]cyclohexanone (>99% ee).

ED Entered STN: 08 Mar 2002

IT **78-94-4**, Methyl vinyl ketone, reactions **930-30-3**, 2-Cyclopentenone **930-68-7**, 2-Cyclohexen-1-one **1121-66-0**, 2-Cycloheptenone
RL: RCT (Reactant); **RACT (Reactant or reagent)**
(preparation of lanthanum-linked bis(BINOL) complexes as catalysts for asym. Michael addition reactions of cyclic or noncyclic enones with β-dicarbonyl compds.)

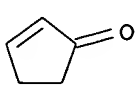
RN 78-94-4 HCAPLUS

CN 3-Buten-2-one (8CI, 9CI) (CA INDEX NAME)



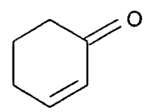
RN 930-30-3 HCAPLUS

CN 2-Cyclopenten-1-one (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

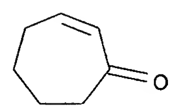


RN 930-68-7 HCAPLUS

CN 2-Cyclohexen-1-one (6CI, 8CI, 9CI) (CA INDEX NAME)

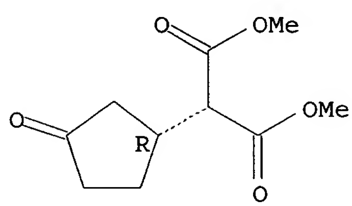


RN 1121-66-0 HCAPLUS
CN 2-Cyclohepten-1-one (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



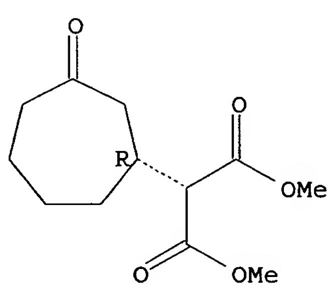
IT **287493-81-6P**, (R)-(+)-3-[Bis(methoxycarbonyl)methyl]cyclop
entanone **287493-82-7P**, (R)-(+)-3-[1,1-
Bis(methoxycarbonyl)methyl]cycloheptanone **403620-79-1P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP
(Preparation); RACT (Reactant or reagent)
(preparation of lanthanum-linked bis(BINOL) complexes as catalysts
for asym. Michael addition reactions of cyclic or noncyclic enones
with β-dicarbonyl compds.)
RN 287493-81-6 HCAPLUS
CN Propanedioic acid, [(1R)-3-oxocyclopentyl]-, dimethyl ester (9CI)
(CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



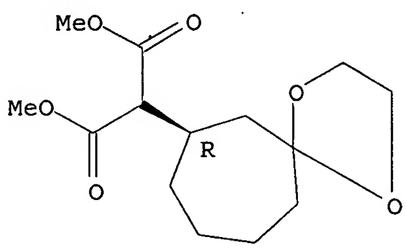
RN 287493-82-7 HCAPLUS
CN Propanedioic acid, [(1R)-3-oxocycloheptyl]-, dimethyl ester (9CI)
(CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



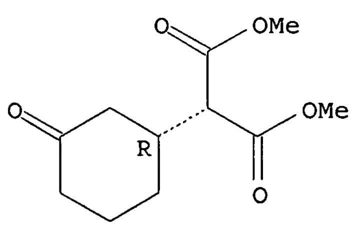
RN 403620-79-1 HCAPLUS
CN Propanedioic acid, (7R)-1,4-dioxaspiro[4.6]undec-7-yl-, dimethyl
ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



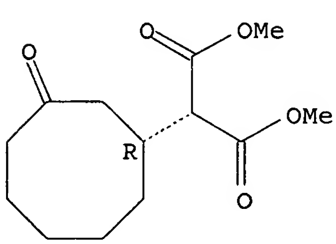
IT 164931-77-5P, (R)-(+)-3-[Bis(methoxycarbonyl)methyl]cycloh
exanone 287493-83-8P, (R)-(-)-3-[1,1-
Bis(methoxycarbonyl)methyl]cyclooctanone 287493-86-1P,
(R)-(-)-2-(Methoxycarbonyl)-3-methyl-5-oxo-5-phenylpentanoic acid
methyl ester 403620-77-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of lanthanum-linked bis(BINOL) complexes as catalysts
for asym. Michael addition reactions of cyclic or noncyclic enones
with β-dicarbonyl compds.)
RN 164931-77-5 HCAPLUS
CN Propanedioic acid, [(1R)-3-oxocyclohexyl]-, dimethyl ester (9CI)
(CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



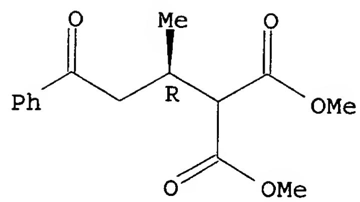
RN 287493-83-8 HCAPLUS
CN Propanedioic acid, [(1R)-3-oxocyclooctyl]-, dimethyl ester (9CI)
(CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



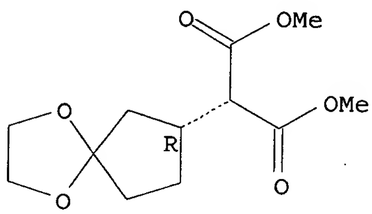
RN 287493-86-1 HCAPLUS
CN Propanedioic acid, [(1R)-1-methyl-3-oxo-3-phenylpropyl]-, dimethyl
ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



RN 403620-77-9 HCAPLUS
CN Propanedioic acid, (7R)-1,4-dioxaspiro[4.4]non-7-yl-, dimethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IC ICM C07F005-00
ICS B01J031-22; C07B053-00; C07C043-178; C07C067-333; C07C069-716; C07C069-757; C07D317-60; C07D317-72; C07B061-00; C07M007-00
CC 78-7 (Inorganic Chemicals and Reactions)
Section cross-reference(s): 24, 25, 28
IT **Asymmetric synthesis and induction**
(preparation of lanthanum-linked bis(BINOL) complexes as catalysts for asym. Michael addition reactions of cyclic or noncyclic enones with β-dicarbonyl compds.)
IT **Michael reaction**
(stereoselective; preparation of lanthanum-linked bis(BINOL) complexes as **catalysts** for asym. Michael addition reactions of cyclic or noncyclic enones with β-dicarbonyl compds.)
IT **78-94-4**, Methyl vinyl ketone, reactions 108-59-8, Dimethyl malonate 126-39-6, 2-Ethyl-2-methyl-1,3-dioxolane **930-30-3**, 2-Cyclopentenone **930-68-7**, 2-Cyclohexen-1-one **1121-66-0**, 2-Cycloheptenone 1195-60-4, 2-Cyclononenone 1655-07-8, Ethyl 2-oxocyclohexanecarboxylate 1728-25-2, 2-Cyclooctenone 15014-25-2, Dibenzyl malonate 19446-52-7, Lanthanum isopropoxide 35845-66-0 82794-36-3, Dibenzyl methylmalonate
RL: RCT (Reactant); **RACT (Reactant or reagent)**
(preparation of lanthanum-linked bis(BINOL) complexes as catalysts for asym. Michael addition reactions of cyclic or noncyclic enones with β-dicarbonyl compds.)
IT 185760-71-8P, (R)-(+)-3-[Bis(benzyloxycarbonyl)methyl]cyclopentanone 185760-72-9P, (R)-(+)-3-[Bis(benzyloxycarbonyl)methyl]cycloheptanone **287493-81-6P**, (R)-(+)-3-[Bis(methoxycarbonyl)methyl]cyclopentanone **287493-82-7P**, (R)-(+)-3-[1,1-Bis(methoxycarbonyl)methyl]cycloheptanone **403620-79-1P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP

(Preparation); RACT (Reactant or reagent)
(preparation of lanthanum-linked bis(BINOL) complexes as catalysts for asym. Michael addition reactions of cyclic or noncyclic enones with β-dicarbonyl compds.)

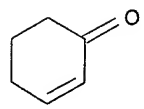
IT 69881-57-8P, (R)-(+)-2-Oxo-1-(3-oxobutyl)cyclohexane-1-carboxylic acid ethyl ester 164931-75-3P, (R)-(+)-3-[Bis(benzyloxycarbonyl)methyl]cyclohexanone 164931-76-4P, (R)-(+)-3-[1,1-Bis(benzyloxycarbonyl)ethyl]cyclohexanone **164931-77-5P**, (R)-(+)-3-[Bis(methoxycarbonyl)methyl]cyclohexanone **287493-83-8P**, (R)-(-)-3-[1,1-Bis(methoxycarbonyl)methyl]cyclooctanone 287493-84-9P, (R)-(-)-3-[1,1-Bis(benzyloxycarbonyl)methyl]cyclononanone 287493-85-0P, (R)-(-)-2-(Benzyloxycarbonyl)-3-methyl-5-oxo-5-phenylpentanoic acid benzyl ester **287493-86-1P**, (R)-(-)-2-(Methoxycarbonyl)-3-methyl-5-oxo-5-phenylpentanoic acid methyl ester 403620-76-8P **403620-77-9P** 403620-78-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of lanthanum-linked bis(BINOL) complexes as catalysts for asym. Michael addition reactions of cyclic or noncyclic enones with β-dicarbonyl compds.)

L93 ANSWER 17 OF 34 HCAPLUS

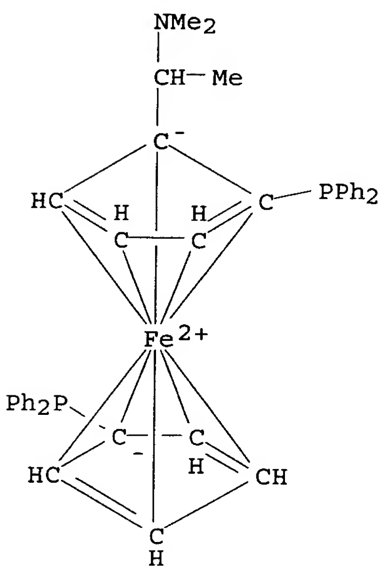
ACCESSION NUMBER: 2002:153736 HCAPLUS
DOCUMENT NUMBER: 137:169294
TITLE: Efficient Mukaiyama aldol reaction by silver(I) carboxylate-bis(phosphine) catalysts
AUTHOR(S): Ohkouchi, Munetaka; Masui, Dai; Yamaguchi, Motowo; Yamagishi, Takamichi
CORPORATE SOURCE: Department of Applied Chemistry, Graduate School of Engineering, Tokyo Metropolitan University, Hachioji-shi, 192-0397, Japan
SOURCE: Nippon Kagaku Kaishi (**2002**), (2), 223-229
CODEN: NKAKB8; ISSN: 0369-4577
PUBLISHER: Nippon Kagakkai
DOCUMENT TYPE: Journal
LANGUAGE: Japanese
OTHER SOURCE(S): CASREACT 137:169294

AB Silver(I) carboxylate-BINAP complex, water tolerant and air-stable, is a highly efficient catalyst for Mukaiyama aldol reaction using silyl enol ethers or ketene silyl acetals as nucleophiles. The Mukaiyama aldol reaction of aldehydes or keto esters in DMF afforded aldol products quant. in a short reaction time by this silver(I) carboxylate-BINAP catalyst. Using ketene silyl acetals, aliphatic ketones also gave the aldol products in high yields, however, with aromatic ketones both aldol reaction and silyl transfer reaction were observed The silver(I) carboxylate-BINAP catalyst acts as a good catalyst for Mukaiyama Michael addition of α,β-unsatd. ketones. The catalyst strongly activates nucleophiles to cause the aldol reaction easily.

ED Entered STN: 28 Feb 2002
IT **930-68-7**, 2-Cyclohexenone **74311-56-1**, (S)-(R)-BPPFA
RL: RCT (Reactant); **RACT (Reactant or reagent)**
(efficient Mukaiyama aldol reaction or Mukaiyama Michael addition by silver(I) carboxylate-bis(phosphine) catalysts)
RN 930-68-7 HCAPLUS
CN 2-Cyclohexen-1-one (6CI, 8CI, 9CI) (CA INDEX NAME)



RN 74311-56-1 HCAPLUS
CN Ferrocene, 1-[(1R)-1-(dimethylamino)ethyl]-1',2-bis(diphenylphosphino)-, (2S)- (9CI) (CA INDEX NAME)



CC 25-18 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
Section cross-reference(s): 78
IT **Asymmetric synthesis and induction**
Michael reaction
Michael reaction catalysts
(efficient Mukaiyama aldol reaction or Mukaiyama Michael addition by silver(I) carboxylate-bis(phosphine) **catalysts**)
IT 66-77-3, 1-Naphthaldehyde 66-99-9, 2-Naphthaldehyde 67-64-1, Acetone, reactions 98-86-2, Acetophenone, reactions 100-06-1, p-Methoxyacetophenone 100-19-6, p-Nitroacetophenone 100-52-7, Benzaldehyde, reactions 108-94-1, Cyclohexanone, reactions 110-62-3, Butyraldehyde 134-81-6, Benzil 563-63-3, Silver(I) acetate 600-22-6, Methyl pyruvate 614-47-1 709-63-7, p-Trifluoromethylacetophenone **930-68-7**, 2-Cyclohexenone 1896-62-4 6651-36-1 6737-42-4, DPPP 7688-25-7, DPPB 13735-81-4, Acetophenone trimethylsilyl enol ether 14371-10-9, trans-Cinnamaldehyde 15206-55-0, Methyl phenyloxoacetate 31469-15-5 31469-16-6 37002-48-5, (S,S)-DIOP 66323-99-7 **74311-56-1**, (S)-(R)-BPPFA 76189-56-5, (S)-BINAP 100165-88-6, (S)-Tol-BINAP
RL: RCT (Reactant); **RACT (Reactant or reagent)**
(efficient Mukaiyama aldol reaction or Mukaiyama Michael addition by silver(I) carboxylate-bis(phosphine) catalysts)

L93 ANSWER 18 OF 34 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2001:420228 HCAPLUS

DOCUMENT NUMBER: 135:241689
TITLE: Catalytic asymmetric Michael reactions using a chiral rhodium complex
AUTHOR(S): Suzuki, T.; Torii, T.
CORPORATE SOURCE: Graduate School of Pharmaceutical Sciences, The University of Tokyo, Tokyo, Bunkyo-ku, Hongo, 113-0033, Japan
SOURCE: Tetrahedron: Asymmetry (**2001**), 12(7), 1077-1081
CODEN: TASYE3; ISSN: 0957-4166
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 135:241689

AB Catalytic asym. Michael reaction of β-keto esters and Me vinyl ketone was achieved using a chiral diamine-based Rh complex to give the Michael adducts in up to 75% e.e.

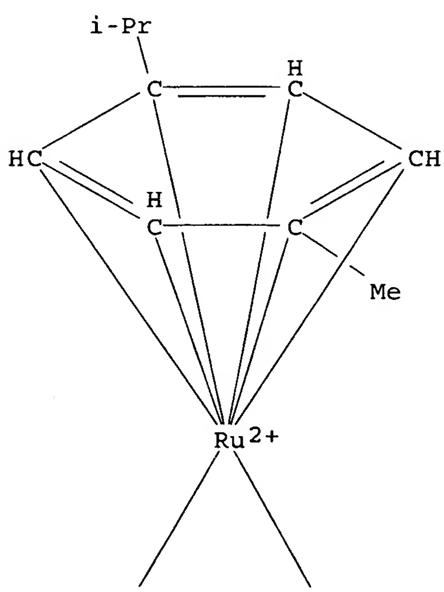
ED Entered STN: 11 Jun 2001

IT **195516-84-8**
RL: CAT (Catalyst use); USES (Uses)
(asym. Michael reaction catalyzed by chiral rhodium complex)

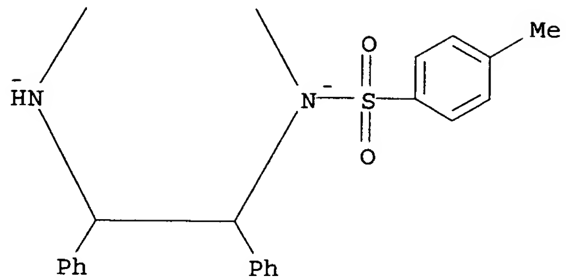
RN 195516-84-8 HCAPLUS

CN Ruthenium, [N-[(1R,2R)-2-amino-1,2-diphenylethyl]-4-methylbenzenesulfonamidato(2-)-κN][(1,2,3,4,5,6-η)-1-methyl-4-(1-methylethyl)benzene]- (9CI) (CA INDEX NAME)

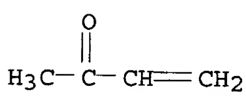
PAGE 1-A



PAGE 2-A

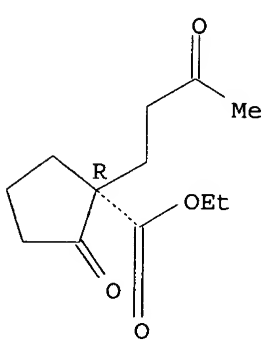


IT 78-94-4, Methyl vinyl ketone, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(asym. Michael reaction catalyzed by chiral rhodium complex)
RN 78-94-4 HCAPLUS
CN 3-Buten-2-one (8CI, 9CI) (CA INDEX NAME)



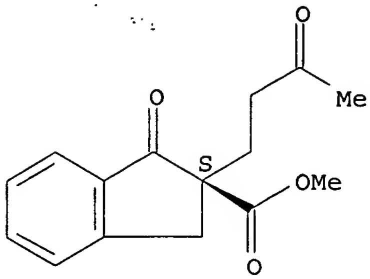
IT **58623-79-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(asym. Michael reaction catalyzed by chiral rhodium complex)
RN 58623-79-3 HCAPLUS
CN Cyclopentanecarboxylic acid, 2-oxo-1-(3-oxobutyl)-, ethyl ester, (1R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



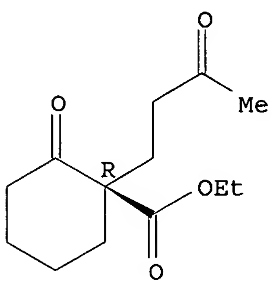
IT **58623-84-0P 69881-57-8P 78044-62-9P**
360795-53-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(asym. Michael reaction catalyzed by chiral rhodium complex)
RN 58623-84-0 HCAPLUS
CN 1H-Indene-2-carboxylic acid, 2,3-dihydro-1-oxo-2-(3-oxobutyl)-, methyl ester, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



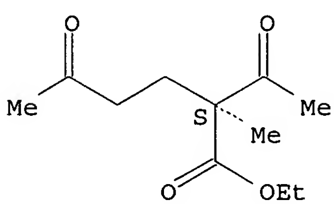
RN 69881-57-8 HCAPLUS
CN Cyclohexanecarboxylic acid, 2-oxo-1-(3-oxobutyl)-, ethyl ester, (1R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



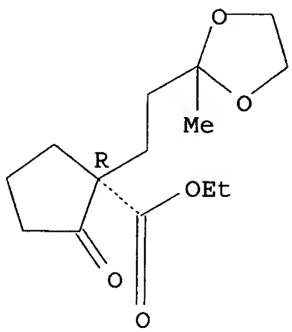
RN 78044-62-9 HCAPLUS
CN Hexanoic acid, 2-acetyl-2-methyl-5-oxo-, ethyl ester, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



RN 360795-53-5 HCAPLUS
CN Cyclopentanecarboxylic acid, 1-[2-(2-methyl-1,3-dioxolan-2-yl)ethyl]-2-oxo-, ethyl ester, (1R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



CC 21-2 (General Organic Chemistry)
IT **Michael reaction**
  Michael reaction catalysts
  (stereoselective; asym. Michael reaction catalyzed by chiral rhodium complex)
IT 12354-84-6 12354-85-7 52462-29-0 78615-08-4 144222-34-4
195516-84-8 360795-52-4
RL: CAT (Catalyst use); USES (Uses)
  (asym. Michael reaction catalyzed by chiral rhodium complex)
IT **78-94-4**, Methyl vinyl ketone, reactions 609-14-3
611-10-9 1655-07-8 22955-77-7
RL: RCT (Reactant); RACT (Reactant or reagent)
  (asym. Michael reaction catalyzed by chiral rhodium complex)
IT **58623-79-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
  (asym. Michael reaction catalyzed by chiral rhodium complex)
IT **58623-84-0P 69881-57-8P 78044-62-9P**
360795-53-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
  (asym. Michael reaction catalyzed by chiral rhodium complex)
REFERENCE COUNT: 48 THERE ARE 48 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L93 ANSWER 19 OF 34 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2001:12419 HCAPLUS
DOCUMENT NUMBER: 134:86044
TITLE: Preparation of chiral 2-amino-2'-diphenylphosphino-1,1'-binaphthyl derivatives as metal catalyst ligands
INVENTOR(S): Zhang, Xumu
PATENT ASSIGNEE(S): The Penn State Research Foundation, USA
SOURCE: PCT Int. Appl., 93 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001000581	A1	20010104	WO 2000-US17903	2000

0629
<--
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN,
CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM,
HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK,
LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ,
PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT,
TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD,
RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE,
CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL,
PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE,
SN, TD, TG
US 6380392 B1 20020430 US 2000-607005
2000
0629
<--
PRIORITY APPLN. INFO.: US 1999-141795P P
1999
0630
<--
OTHER SOURCE(S): CASREACT 134:86044; MARPAT 134:86044

AB Title ligands are bidentate, tridentate, tetradentate, or pentadentate and include P-P, P-N, N-N, mixed P-N, Schiff base or carbene sites. Transition metal complexes with these ligands are effective catalysts for asym. reactions. Thus, Et2Zn addition to 2-cyclohexenone in the presence of (S)-2-(2-pyridinylcarbonylamino)-2'-diphenylphosphino-1,1'-binaphthyl complex with Cu gave (S)-3-ethylcyclohexanone of 92% ee with 98% conversion.

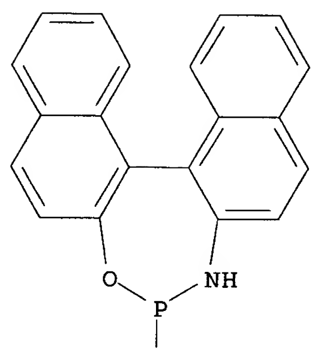
ED Entered STN: 05 Jan 2001

IT **316831-08-0P**
RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(preparation of chiral 2-amino-2'-diphenylphosphino-1,1'-binaphthyl derivs. as metal catalyst ligands)

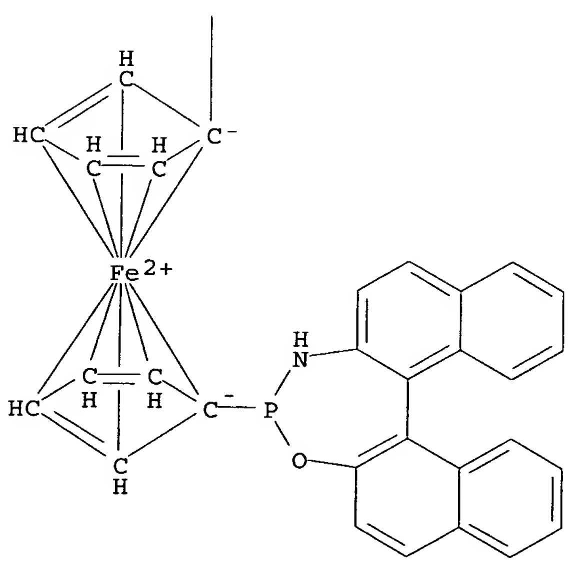
RN 316831-08-0 HCAPLUS

CN Ferrocene, 1,1'-bis(dinaphth[2,1-d:1',2'-f][1,3,2]oxazaphosphepin-4(5H)-yl)- (9CI) (CA INDEX NAME)

PAGE 1-A

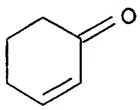


PAGE 2-A



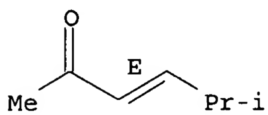
IT 930-68-7, 2-Cyclohexenone **1821-29-0**,
(E)-5-Methyl-3-hexen-2-one
RL: RCT (Reactant); **RACT (Reactant or reagent)**
(preparation of chiral 2-amino-2'-diphenylphosphino-1,1'-binaphthyl derivs. as metal catalyst ligands)
RN 930-68-7 HCAPLUS

CN 2-Cyclohexen-1-one (6CI, 8CI, 9CI) (CA INDEX NAME)



RN 1821-29-0 HCAPLUS
CN 3-Hexen-2-one, 5-methyl-, (3E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



IC ICM C07D213-81
ICS C07D237-20; C07D307-52; C07D333-38; C07F009-53
CC 25-24 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
Section cross-reference(s): 21
IT **Asymmetric synthesis and induction**
(preparation of chiral 2-amino-2'-diphenylphosphino-1,1'-binaphthyl derivs. as metal catalyst ligands)
IT **Michael reaction**
(stereoselective, **catalysts**; preparation of chiral 2-amino-2'-diphenylphosphino-1,1'-binaphthyl derivs. as metal catalyst ligands)
IT 259260-34-9P 259260-35-0P 316811-92-4P 316811-94-6P
316811-96-8P 316811-98-0P 316812-00-7P 316812-03-0P
316812-05-2P 316812-07-4P 316812-09-6P 316812-11-0P
316812-13-2P 316812-15-4P 316812-17-6P 316812-19-8P
316812-21-2P 316812-23-4P 316812-25-6P 316812-27-8P
316812-29-0P 316812-31-4P 316812-33-6P 316812-35-8P
316812-37-0P 316812-39-2P 316812-41-6P 316812-43-8P
316812-45-0P 316812-47-2P 316812-49-4P 316812-51-8P
316812-53-0P 316812-56-3P 316812-59-6P 316812-61-0P
316812-63-2P 316812-65-4P 316812-67-6P 316812-69-8P
316812-71-2P 316812-72-3P 316812-73-4P 316812-74-5P
316812-75-6P **316831-08-0P** 317330-09-9P 317330-10-2P
317330-11-3P 317330-12-4P 317330-13-5P 317330-14-6P
317330-15-7P 317330-16-8P 317330-17-9P 317330-18-0P
317330-19-1P 317330-79-3P
RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(preparation of chiral 2-amino-2'-diphenylphosphino-1,1'-binaphthyl derivs. as metal catalyst ligands)
IT 98-98-6, 2-Pyridinecarboxylic acid 100-42-5, Styrene, reactions 135-19-3, 2-Naphthol, reactions 602-09-5, 1,1'-Bi-2-naphthol 614-47-1, trans-1,3-Diphenyl-2-propen-1-one 623-73-4, Ethyl diazoacetate **930-68-7**, 2-Cyclohexenone 934-60-1, 2-Carboxy-6-methylpyridine 1013-88-3, Iminodiphenylmethane 1121-60-4, 2-Pyridinecarboxaldehyde 1122-72-1, 6-Methyl-2-Pyridinecarboxaldehyde 1195-59-1, 2,6-Pyridinedimethanol **1821-29-0**, (E)-5-Methyl-3-hexen-2-one 1896-62-4, (E)-4-Phenyl-3-buten-2-one 3739-94-4,

2,6-Pyridinedicarbonyl chloride 4559-70-0, Diphenylphosphine oxide 22252-15-9, (E)-3-(4-Methoxyphenyl)-1-phenyl-2-propen-1-one 22252-16-0, (E)-3-(4-Chlorophenyl)-1-phenyl-2-propen-1-one 22966-19-4, (E)-1-(4-Methoxyphenyl)-3-phenyl-2-propen-1-one 22966-22-9, (E)-1-(4-Chlorophenyl)-3-phenyl-2-propen-1-one 37942-07-7, 3,5-Di-tert-butyl-2-hydroxybenzaldehyde
RL: RCT (Reactant); **RACT (Reactant or reagent)**
(preparation of chiral 2-amino-2'-diphenylphosphino-1,1'-binaphthyl derivs. as metal catalyst ligands)

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

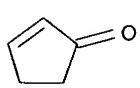
L93 ANSWER 20 OF 34 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2000:845259 HCAPLUS
DOCUMENT NUMBER: 134:131299
TITLE: Immobilization of asymmetric multifunctional catalysts on an insoluble polymer
AUTHOR(S): Matsunaga, Shigeki; Ohshima, Takashi; Shibasaki, Masakatsu
CORPORATE SOURCE: Graduate School of Pharmaceutical Sciences, The University of Tokyo, Tokyo, 113-0033, Japan
SOURCE: Tetrahedron Letters (**2000**), 41(44), 8473-8478
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 134:131299

AB A polymer-supported linked-BINOL was synthesized to immobilize asym. catalysts with two BINOL units. The advantage of the polymer-supported linked-BINOL over randomly polymer-supported BINOL was confirmed by asym. Michael reaction. A novel polymer-supported La-Zn-linked-BINOL complex afforded the Michael adduct in good yield and moderate ee.

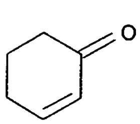
ED Entered STN: 05 Dec 2000

IT **930-30-3**, 2-Cyclopentenone **930-68-7**, 2-Cyclohexenone **1121-66-0**, 2-Cycloheptenone
RL: RCT (Reactant); **RACT (Reactant or reagent)**
(asym. Michael reaction catalyzed by lanthanum binaphthalenediol complex)

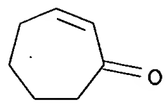
RN 930-30-3 HCAPLUS
CN 2-Cyclopenten-1-one (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



RN 930-68-7 HCAPLUS
CN 2-Cyclohexen-1-one (6CI, 8CI, 9CI) (CA INDEX NAME)

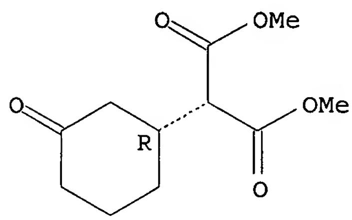


RN 1121-66-0 HCAPLUS
CN 2-Cyclohepten-1-one (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



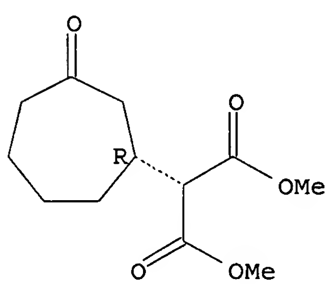
IT **164931-77-5P 287493-82-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(asym. Michael reaction catalyzed by lanthanum binaphthalenediol complex)
RN 164931-77-5 HCAPLUS
CN Propanedioic acid, [(1R)-3-oxocyclohexyl]-, dimethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



RN 287493-82-7 HCAPLUS
CN Propanedioic acid, [(1R)-3-oxocycloheptyl]-, dimethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



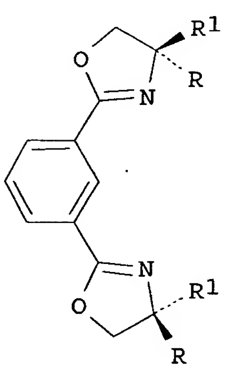
CC 25-24 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
Section cross-reference(s): 67, 78
IT **Asymmetric synthesis and induction**
(preparation of polymer-supported binaphthalenediol dimer as asym. Michael catalyst)
IT **Michael reaction**
Michael reaction catalysts
(stereoselective; preparation of polymer-supported binaphthalenediol dimer as asym. Michael catalyst)
IT 108-59-8, Dimethyl malonate **930-30-3**, 2-Cyclopentenone

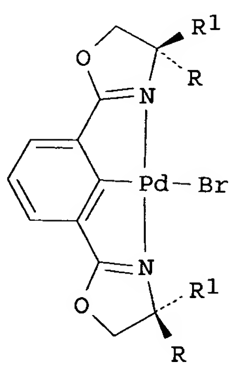
930-68-7, 2-Cyclohexenone **1121-66-0**,
2-Cycloheptenone 15014-25-2, Dibenzyl malonate
RL: RCT (Reactant); **RACT (Reactant or reagent)**
(asym. Michael reaction catalyzed by lanthanum binaphthalenediol complex)

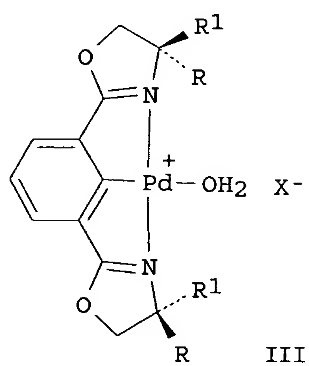
IT 164931-75-3P **164931-77-5P** 185760-71-8P 185760-72-9P **287493-82-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(asym. Michael reaction catalyzed by lanthanum binaphthalenediol complex)

REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L93 ANSWER 21 OF 34 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2000:145263 HCAPLUS
DOCUMENT NUMBER: 132:308474
TITLE: Cationic [2,6-Bis(2'-oxazolinyl)phenyl]palladium(II) Complexes: Catalysts for the Asymmetric Michael Reaction
AUTHOR(S): Stark, Mark A.; Jones, Geraint; Richards, Christopher J.
CORPORATE SOURCE: Department of Chemistry, Cardiff University, Cardiff, CF10 3TB, UK
SOURCE: Organometallics (**2000**), 19(7), 1282-1291
CODEN: ORGND7; ISSN: 0276-7333
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 132:308474
GI


I


II


III

AB Reaction of 1,3-dicyanobenzene with β-amino alcs. (S)-H2NCHRCH2OH (R = iPr, iBu, tBu, CH2Cy, CH2Ph) and (R)-H2NCHPhCH2OH gave new 1,3-bis(2-oxazolin-2-yl)benzenes (I; R = R1 = Me; R = iPr, iBu, tBu, CH2Cy, CH2Ph, R1 = H; R = H, R1 = Ph) (30-51%). These, together with 1,3-bis(4,4-dimethyl-2-oxazolin-2-yl)benzene, were treated with LDA/TMEDA followed by the addition of PdBr2(1,5-COD) to give [2,6-bis(2-oxazolin-2-yl)phenyl]palladium(II) bromide complexes (II; R = R1 = Me; R =

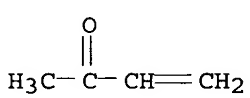
iPr, iBu, tBu, CH2Cy R1 = H (Cy = cyclohexyl)) (21-41%). In two cases no complexes were obtained (with reactant I; R = H, R1 = Ph; R = CH2Ph, R1 = H) due to ring opening of the oxazolines by LDA/TMEDA. Treatment of the Pd complexes II with AgBF4, AgOTf, or AgSbF6 in wet CH2Cl2 provided cationic [2,6-bis(2-oxazolin-2-yl)phenyl]palladium complexes (III; R, R1 same as above, X- = BF4-, F3CSO3-, SbF6-)(28-87%) containing H2O coordinated to Pd, as established by an x-ray crystal structure anal. of (S,S)-[2,6-bis(4-isopropyl-2-oxazolin-2-yl)phenyl]aquopalladium(II) trifluoromethanesulfonate (III; R = iPr, R1 = H, X = F3CSO3-). All of the cationic complexes proved to be efficient catalysts for the Michael reaction between α-cyanocarboxylates and Me vinyl ketone and between acrylonitrile and activated Michael donors. Selectivities of up to 34% ee were obtained for the formation of (R)-Et 2-cyano-2-methyl-5-oxohexanoate.

ED Entered STN: 05 Mar 2000

IT **78-94-4**, 3-Buten-2-one, reactions
RL: RCT (Reactant); **RACT (Reactant or reagent)**
([bis(oxazolinyl)phenyl]palladium(II) cationic complex-catalyzed asym. Michael reaction of)

RN 78-94-4 HCAPLUS

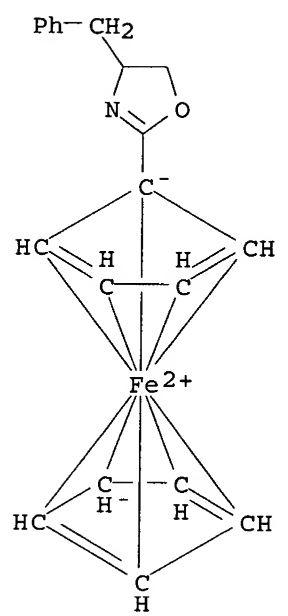
CN 3-Buten-2-one (8CI, 9CI) (CA INDEX NAME)



IT **162157-05-3**, (S)-2-Ferrocenyl-4-benzyl-2-oxazoline
RL: RCT (Reactant); RACT (Reactant or reagent)
(benzylic deprotonation followed by reaction with acid)

RN 162157-05-3 HCAPLUS

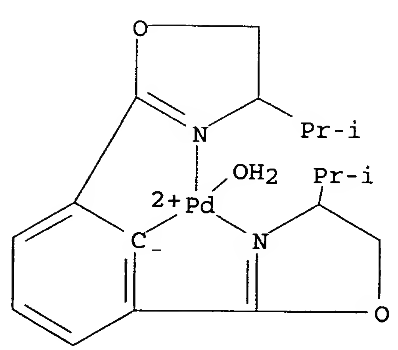
CN Ferrocene, [(4S)-4,5-dihydro-4-(phenylmethyl)-2-oxazolyl]- (9CI) (CA INDEX NAME)



IT 196207-76-8P
RL: CAT (Catalyst use); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(crystal structure; preparation of cationic [bis(oxazolinyl)phenyl]palladium(II) complexes as catalysts for asym. Michael reaction)
RN 196207-76-8 HCAPLUS
CN Palladium(1+), aqua[2,6-bis[(4S,4'S)-4,5-dihydro-4-(1-methylethyl)-2-oxazolyl-κN3]phenyl-κC]-, (SP-4-3)-, salt with trifluoromethanesulfonic acid (1:1) (9CI) (CA INDEX NAME)

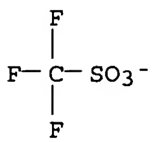
CM 1

CRN 196207-75-7
CMF C18 H25 N2 O3 Pd
CCI CCS



CM 2

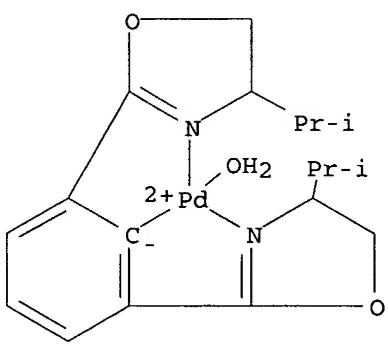
CRN 37181-39-8
CMF C F3 O3 S



IT **196207-77-9P**
RL: CAT (Catalyst use); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation as catalyst for asym. Michael reaction and substitution reaction with nitriles)
RN 196207-77-9 HCAPLUS
CN Palladium(1+), aqua[2,6-bis[(4S,4'S)-4,5-dihydro-4-(1-methylethyl)-2-oxazolyl-κN3]phenyl-κC]-, (SP-4-3)-, (OC-6-11)-hexafluoroantimonate(1-) (9CI) (CA INDEX NAME)

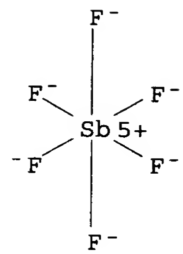
CM 1

CRN 196207-75-7
CMF C18 H25 N2 O3 Pd
CCI CCS

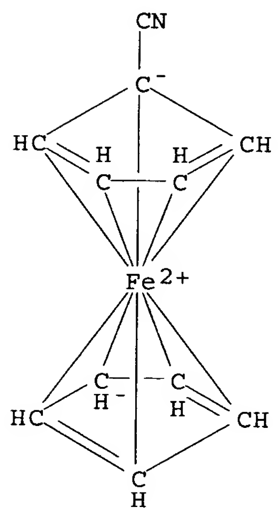


CM 2

CRN 17111-95-4
CMF F6 Sb
CCI CCS



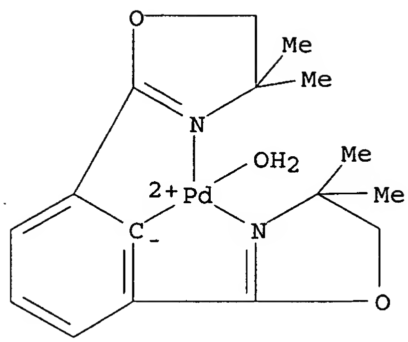
IT 1273-84-3P, Ferrocenyl cyanide 196207-74-6P
265127-72-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 1273-84-3 HCAPLUS
CN Ferrocene, cyano- (9CI) (CA INDEX NAME)



RN 196207-74-6 HCAPLUS
CN Palladium(1+), aqua[2,6-bis(4,5-dihydro-4,4-dimethyl-2-oxazolyl-κN3)phenyl-κC]-, (SP-4-3)-, tetrafluoroborate(1-) (9CI) (CA INDEX NAME)

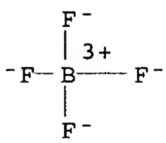
CM 1

CRN 196207-73-5
CMF C16 H21 N2 O3 Pd
CCI CCS



CM 2

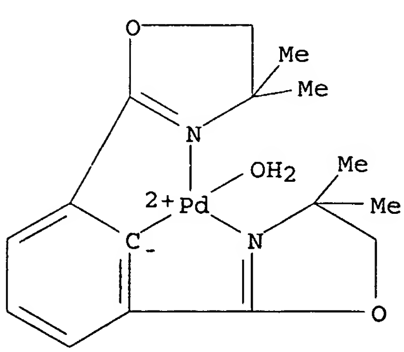
CRN 14874-70-5
CMF B F4
CCI CCS



RN 265127-72-8 HCAPLUS
CN Palladium(1+), aqua[2,6-bis(4,5-dihydro-4,4-dimethyl-2-oxazolyl-κN3)phenyl-κC]-, (SP-4-3)-, salt with trifluoromethanesulfonic acid (1:1) (9CI) (CA INDEX NAME)

CM 1

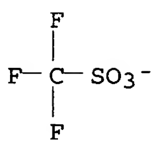
CRN 196207-73-5
CMF C16 H21 N2 O3 Pd
CCI CCS



CM 2

CRN 37181-39-8

CMF C F3 O3 S



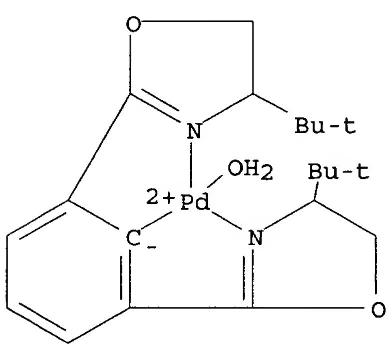
IT **196207-80-4P 196207-82-6P 265127-73-9P**
265127-74-0P 265127-76-2P
RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(preparation of cationic [bis(oxazolinyl)phenyl]palladium(II) complexes as catalysts for asym. Michael reaction)

RN 196207-80-4 HCAPLUS

CN Palladium(1+), aqua[2,6-bis[(4S,5S)-4-(1,1-dimethylethyl)-4,5-dihydro-2-oxazolyl-κN3]phenyl-κC]-, (SP-4-3)-, (OC-6-11)-hexafluoroantimonate(1-) (9CI) (CA INDEX NAME)

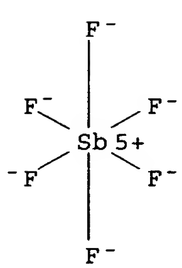
CM 1

CRN 196207-79-1
CMF C20 H29 N2 O3 Pd
CCI CCS



CM 2

CRN 17111-95-4
CMF F6 Sb
CCI CCS

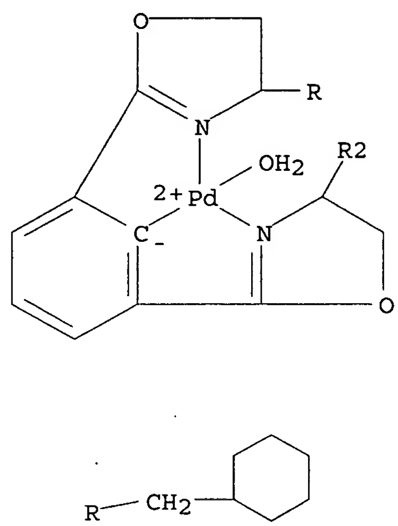


RN 196207-82-6 HCAPLUS
CN Palladium(1+), aqua[2,6-bis[(4S)-4-(cyclohexylmethyl)-4,5-dihydro-2-oxazolyl-κN3]phenyl-κC]-, (SP-4-3)-, (OC-6-11)-hexafluoroantimonate(1-) (9CI) (CA INDEX NAME)

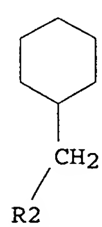
CM 1

CRN 196207-81-5
CMF C26 H37 N2 O3 Pd
CCI CCS

PAGE 1-A

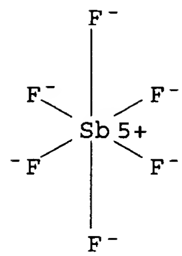


PAGE 2-A



CM 2

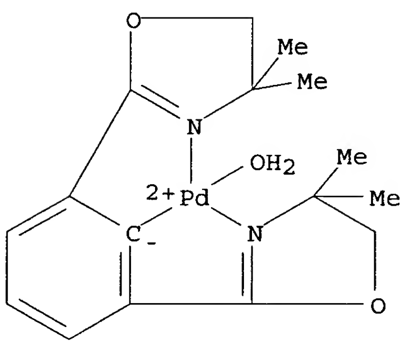
CRN 17111-95-4
CMF F6 Sb
CCI CCS



RN 265127-73-9 HCAPLUS
CN Palladium(1+), aqua[2,6-bis(4,5-dihydro-4,4-dimethyl-2-oxazolyl-κN3)phenyl-κC]-, (SP-4-3)-, (OC-6-11)-hexafluoroantimonate(1-) (9CI) (CA INDEX NAME)

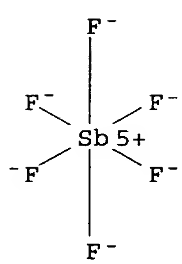
CM 1

CRN 196207-73-5
CMF C16 H21 N2 O3 Pd
CCI CCS



CM 2

CRN 17111-95-4
CMF F6 Sb
CCI CCS

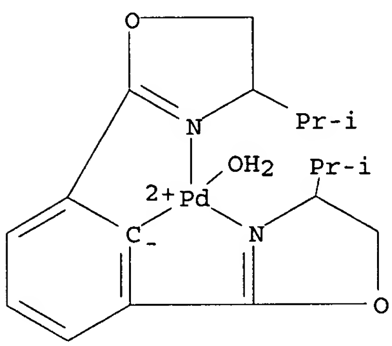


RN 265127-74-0 HCAPLUS
CN Palladium(1+), aqua[2,6-bis[(4S)-4,5-dihydro-4-(1-methylethyl)-2-oxazolyl-κN3]phenyl-κC]-, (SP-4-3)-,

tetrafluoroborate(1-) (9CI) (CA INDEX NAME)

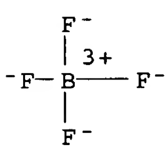
CM 1

CRN 196207-75-7
CMF C18 H25 N2 O3 Pd
CCI CCS



CM 2

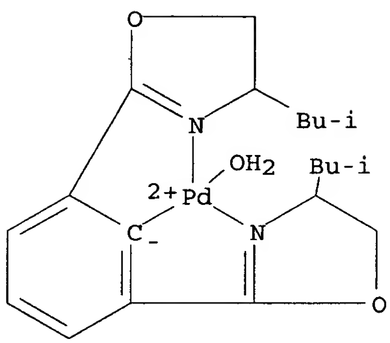
CRN 14874-70-5
CMF B F4
CCI CCS



RN 265127-76-2 HCAPLUS
CN Palladium(1+), aqua[2,6-bis[(4S)-4,5-dihydro-4-(2-methylpropyl)-2-oxazolyl-κN3]phenyl-κC]-, (SP-4-3)-, (OC-6-11)-hexafluoroantimonate(1-) (9CI) (CA INDEX NAME)

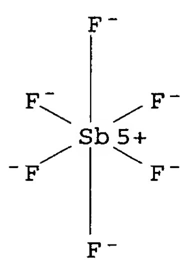
CM 1

CRN 265127-75-1
CMF C20 H29 N2 O3 Pd
CCI CCS

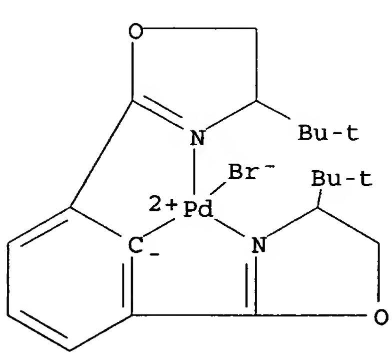


CM 2

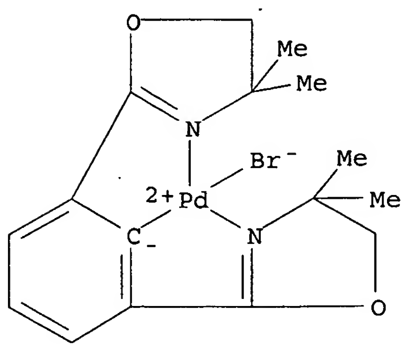
CRN 17111-95-4
CMF F6 Sb
CCI CCS



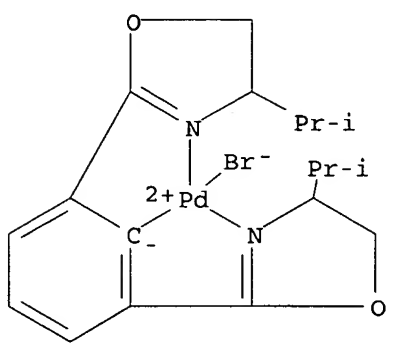
IT **189632-52-8P 196207-70-2P 196207-71-3P**
196207-72-4P 265127-67-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of cationic palladium bis(oxazolinyl)benzene aquo complexes from)
RN 189632-52-8 HCAPLUS
CN Palladium, [2,6-bis[(4S)-4-(1,1-dimethylethyl)-4,5-dihydro-2-oxazolyl-κN3]phenyl-κC]bromo-, (SP-4-3)- (9CI) (CA INDEX NAME)



RN 196207-70-2 HCAPLUS
CN Palladium, [2,6-bis(4,5-dihydro-4,4-dimethyl-2-oxazolyl-κN3)phenyl-κC]bromo-, (SP-4-3)- (9CI) (CA INDEX NAME)



RN 196207-71-3 HCAPLUS
CN Palladium, [2,6-bis[(4S)-4,5-dihydro-4-(1-methylethyl)-2-oxazolyl-κN3]phenyl-κC]bromo-, (SP-4-3)- (9CI) (CA INDEX NAME)



RN 196207-72-4 HCAPLUS
CN Palladium, [2,6-bis[(4S)-4-(cyclohexylmethyl)-4,5-dihydro-2-oxazolyl-κN3]phenyl-κC]bromo-, (SP-4-3)- (9CI) (CA INDEX NAME)

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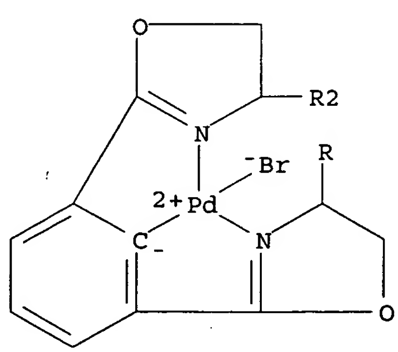
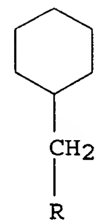
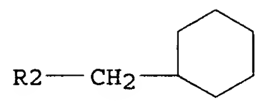
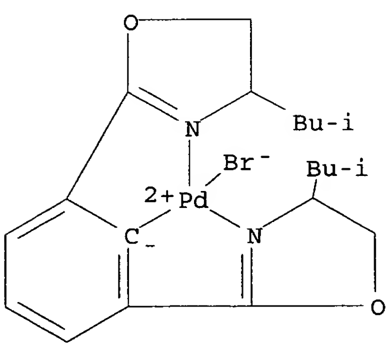


PAGE 2-A





RN 265127-67-1 HCAPLUS
CN Palladium, [2,6-bis[(4S)-4,5-dihydro-4-(2-methylpropyl)-2-oxazolyl-κN3]phenyl-κC]bromo-, (SP-4-3)- (9CI) (CA INDEX NAME)



CC 29-13 (Organometallic and Organometalloidal Compounds)
Section cross-reference(s): 21, 22, 67, 75
IT **Michael reaction catalysts**
(stereoselective; chiral cationic bis(oxazolinyl)palladium(II) complexes as catalysts for asym. Michael reaction)
IT **Michael reaction**
(stereoselective; chiral cationic bis(oxazolinyl)phenylpalladium(II) complexes as **catalysts** for asym. Michael reaction)
IT **Asymmetric synthesis and induction**
(using chiral cationic bis(oxazolinyl)palladium(II) complexes as catalysts for asym. Michael reactions to form chiral products)
IT **78-94-4**, 3-Buten-2-one, reactions 105-56-6, Ethyl cyanoacetate 107-13-1, 2-Propenenitrile, reactions 603-67-8, Diethyl nitromalonate 1572-99-2, Ethyl α-cyanopropionate 66476-82-2, tert-Butyl α-cyanopropionate
RL: RCT (Reactant); **RACT (Reactant or reagent)**
([bis(oxazolinyl)phenyl]palladium(II) cationic complex-catalyzed asym. Michael reaction of)

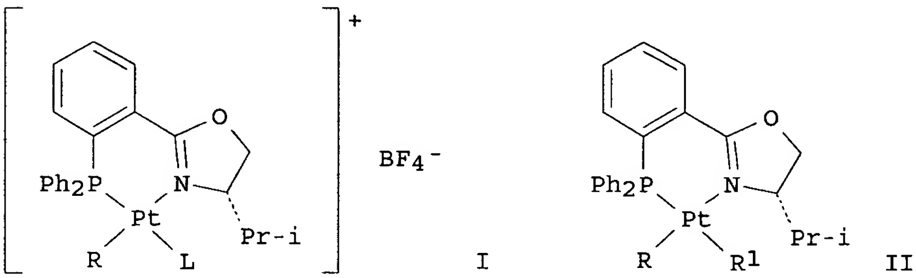
IT 162157-05-3, (S)-2-Ferrocenyl-4-benzyl-2-oxazoline
RL: RCT (Reactant); RACT (Reactant or reagent)
(benzylic deprotonation followed by reaction with acid)
IT 196207-76-8P
RL: CAT (Catalyst use); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(crystal structure; preparation of cationic [bis(oxazolinyl)phenyl]palladium(II) complexes as catalysts for asym. Michael reaction)
IT 196207-77-9P
RL: CAT (Catalyst use); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation as catalyst for asym. Michael reaction and substitution reaction with nitriles)
IT 1273-84-3P, Ferrocenyl cyanide 4407-36-7P, (E)-Cinnamyl alcohol 99170-86-2P, 4,4-Bis(carboethoxy)-4-nitrobutanenitrile 143619-24-3P, (R)-Ethyl 2-cyano-2-methyl-5-oxohexanoate 143619-26-5P, (R)-tert-Butyl 2-cyano-2-methyl-5-oxohexanoate 181186-07-2P, 5-Cyano-5-(carboethoxy)nonane-2,8-dione **196207-74-6P** 265127-68-2P 265127-71-7P, (R,R)-2-Methyl-1,3-bis(4-phenyl-2-oxazolin-2-yl)benzene **265127-72-8P** 265127-80-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
IT **196207-80-4P 196207-82-6P 265127-73-9P 265127-74-0P 265127-76-2P** 265127-78-4P
RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(preparation of cationic [bis(oxazolinyl)phenyl]palladium(II) complexes as catalysts for asym. Michael reaction)
IT **189632-52-8P 196207-70-2P 196207-71-3P 196207-72-4P 265127-67-1P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of cationic palladium bis(oxazolinyl)benzene aquo complexes from)

REFERENCE COUNT: 90 THERE ARE 90 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L93 ANSWER 22 OF 34 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1999:401284 HCAPLUS
DOCUMENT NUMBER: 131:170456
TITLE: Synthesis and Structure of Enantiomerically Pure Platinum Complexes of Phosphino-oxazolines and Their Use in Asymmetric Catalysis
AUTHOR(S): Blacker, A. John; Clarke, Matthew L.; Loft, Michael S.; Mahon, Mary F.; Williams, Jonathan M. J.
CORPORATE SOURCE: Huddersfield Works, Zeneca, Huddersfield, HD2 1FF, UK
SOURCE: Organometallics (**1999**), 18(15), 2867-2873
CODEN: ORGND7; ISSN: 0276-7333
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 131:170456

GI



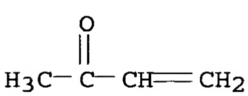
AB Novel organoplatinum complexes of the enantiomerically pure P, N ligand, (4S)-2-[2-(diphenylphosphino)phenyl]-4-isopropyl-1,3-oxazoline (e.g. I; L = ClCH2Cl, R = Me (5a), Ph (5b)), were synthesized and shown to act as Lewis acids. These complexes consist of the bidentate P, N ligand, an achiral organic ligand, and a solvent ligand that can be readily displaced by organic substrates. The solvent ligand is situated cis to the N donor and, as such, is in a chiral pocket created by the oxazoline ring. The complexes are readily prepared from the known, and versatile, precursors (COD)PtR2 (R = Me, Ph) and were obtained as single isomers. Two of the complexes II (R = R1 = Ph (3b); R = Me, R1 = Cl (4a)) have had their structures elucidated by x-ray crystallog. The cationic complexes 5a and 5b are enantioselective catalysts in the Michael reaction of α-cyano carboxylates with Me vinyl ketone. Complex 5a catalyzed the Diels Alder reaction of cyclopentadiene with 2-chloroacrylonitrile to give high conversion to a 7:1 mixture of endo and exo isomers of the resulting adduct with low enantioselectivity (ca. 10% ee).

ED Entered STN: 30 Jun 1999

IT **78-94-4**, Methyl vinyl ketone, reactions
RL: RCT (Reactant); **RACT (Reactant or reagent)**
(asym. Michael reaction with Et cyanopropionate catalyzed by organoplatinum (phosphinophenyl)oxazoline complexes)

RN 78-94-4 HCAPLUS

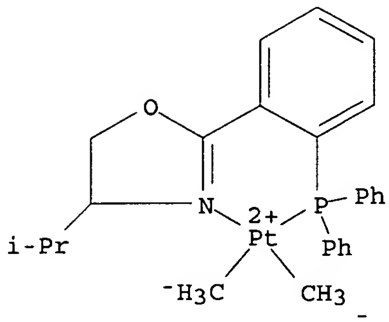
CN 3-Buten-2-one (8CI, 9CI) (CA INDEX NAME)



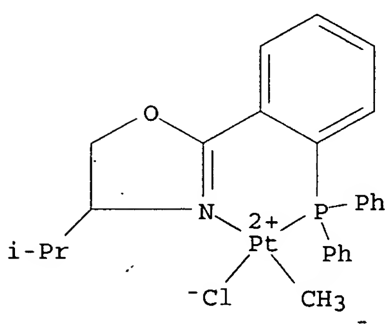
IT **239099-78-6P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and chlorination of)

RN 239099-78-6 HCAPLUS

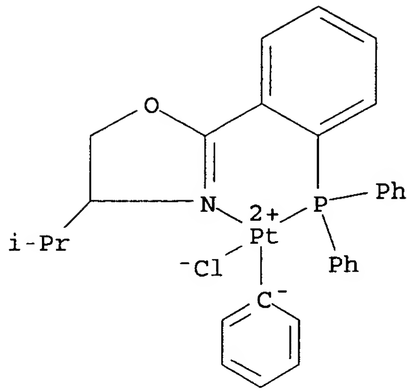
CN Platinum, [(4S)-2-[2-(diphenylphosphino-κP)phenyl]-4,5-dihydro-4-(1-methylethyl)oxazole-κN3]dimethyl-, (SP-4-3)-(9CI) (CA INDEX NAME)



IT 239099-80-0DP, petroleum ether solvate
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and crystal structure of)
RN 239099-80-0 HCAPLUS
CN Platinum, chloro[(4S)-2-[2-(diphenylphosphino-κP)phenyl]-4,5-dihydro-4-(1-methylethyl)oxazole-κN3]methyl-, (SP-4-2)- (9CI) (CA INDEX NAME)



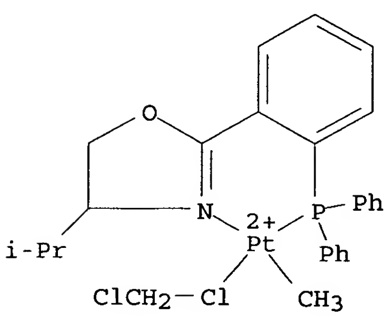
IT **239099-81-1P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction with dichloromethane and silver tetrafluoroborate)
RN 239099-81-1 HCAPLUS
CN Platinum, chloro[(4S)-2-[2-(diphenylphosphino-κP)phenyl]-4,5-dihydro-4-(1-methylethyl)oxazole-κN3]phenyl-, (SP-4-2)- (9CI) (CA INDEX NAME)



IT **239099-83-3P**
RL: CAT (Catalyst use); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation as enantioselective Michael reaction catalysts for reaction of α-cyano carboxylates with Me vinyl ketone)
RN 239099-83-3 HCAPLUS
CN Platinum(1+), [(chloro-κCl)chloromethane][(4S)-2-[2-(diphenylphosphino-κP)phenyl]-4,5-dihydro-4-(1-methylethyl)oxazole-κN3]methyl-, (SP-4-2)-, tetrafluoroborate(1-) (9CI) (CA INDEX NAME)

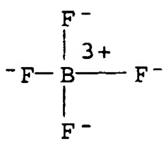
CM 1

CRN 239099-82-2
CMF C26 H29 Cl2 N O P Pt
CCI CCS



CM 2

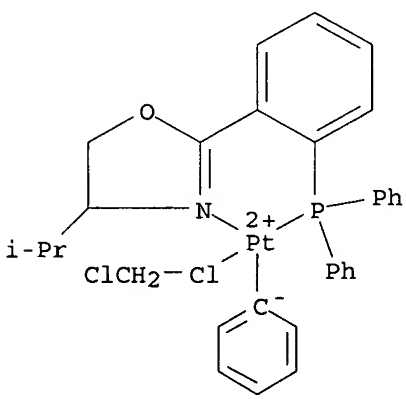
CRN 14874-70-5
CMF B F4
CCI CCS



IT 239099-85-5P
RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(preparation as enantioselective Michael reaction catalysts for reaction of α-cyano carboxylates with Me vinyl ketone)
RN 239099-85-5 HCAPLUS
CN Platinum(1+), [(chloro-κCl)chloromethane][(4S)-2-[2-(diphenylphosphino-κP)phenyl]-4,5-dihydro-4-(1-methylethyl)oxazole-κN3]phenyl-, (SP-4-2)-, tetrafluoroborate(1-) (9CI) (CA INDEX NAME)

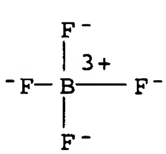
CM 1

CRN 239099-84-4
CMF C31 H31 Cl2 N O P Pt
CCI CCS



CM 2

CRN 14874-70-5
CMF B F4
CCI CCS

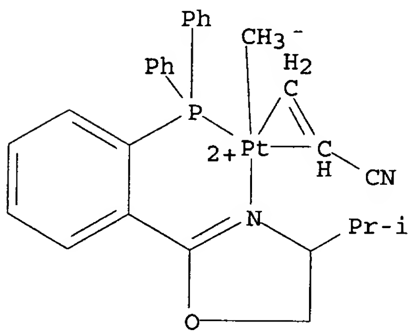


IT 239099-87-7P 239099-89-9P 239099-91-3P
239099-93-5P
RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of)
RN 239099-87-7 HCAPLUS
CN Platinum(1+), [(4S)-2-[2-(diphenylphosphino-κP)phenyl]-4,5-dihydro-4-(1-methylethyl)oxazole-κN3]methyl[(2,3-η)-2-propenenitrile]-, tetrafluoroborate(1-) (9CI) (CA INDEX NAME)

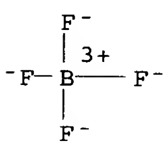
CM 1

CRN 239099-86-6
CMF C28 H30 N2 O P Pt
CCI CCS



CM 2

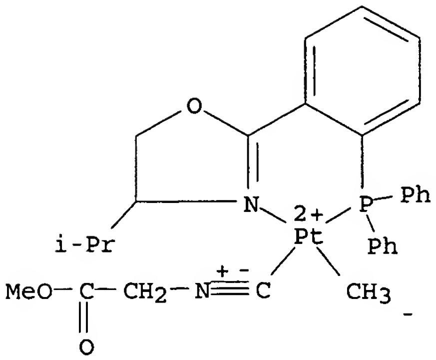
CRN 14874-70-5
CMF B F4
CCI CCS



RN 239099-89-9 HCAPLUS
CN Platinum(1+), [(4S)-2-[2-(diphenylphosphino-κP)phenyl]-4,5-dihydro-4-(1-methylethyl)oxazole-κN3]methyl[methyl (isocyano-κC)acetate]-, (SP-4-3)-, tetrafluoroborate(1-) (9CI) (CA INDEX NAME)

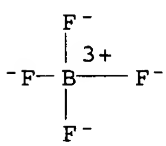
CM 1

CRN 239099-88-8
CMF C29 H32 N2 O3 P Pt
CCI CCS



CM 2

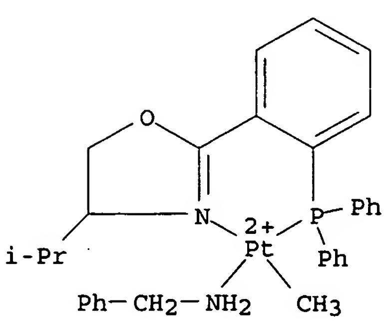
CRN 14874-70-5
CMF B F4
CCI CCS



RN 239099-91-3 HCAPLUS
CN Platinum(1+), (benzenemethanamine)[(4S)-2-[2-(diphenylphosphino-κP)phenyl]-4,5-dihydro-4-(1-methylethyl)oxazole-κN3]methyl-, (SP-4-3)-, tetrafluoroborate(1-) (9CI) (CA INDEX NAME)

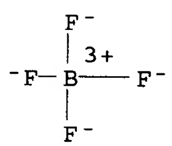
CM 1

CRN 239099-90-2
CMF C32 H36 N2 O P Pt
CCI CCS



CM 2

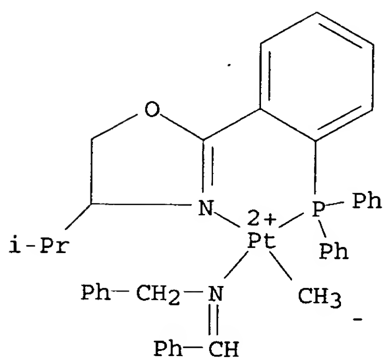
CRN 14874-70-5
CMF B F4
CCI CCS



RN 239099-93-5 HCAPLUS
CN Platinum(1+), [(4S)-2-[2-(diphenylphosphino-κP)phenyl]-4,5-dihydro-4-(1-methylethyl)oxazole-κN3]methyl[N-(phenylmethylene)benzenemethanamine]-, (SP-4-3)-, tetrafluoroborate(1-) (9CI) (CA INDEX NAME)

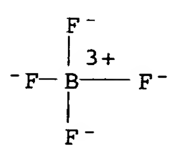
CM 1

CRN 239099-92-4
CMF C39 H40 N2 O P Pt
CCI CCS



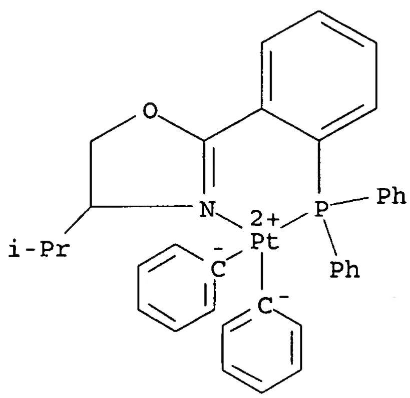
CM 2

CRN 14874-70-5
CMF B F4
CCI CCS

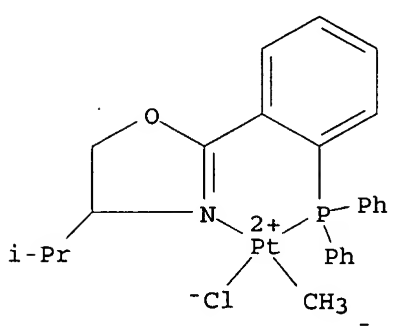


IT **239099-79-7P**
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation, crystal structure, and chlorination of)

RN 239099-79-7 HCAPLUS
CN Platinum, [(4S)-2-[2-(diphenylphosphino-κP)phenyl]-4,5-dihydro-4-(1-methylethyl)oxazole-κN3]diphenyl-, (SP-4-3)-(9CI) (CA INDEX NAME)



IT **239099-80-0P**
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation, mol. structure, and reaction with dichloromethane and silver tetrafluoroborate)
RN 239099-80-0 HCAPLUS
CN Platinum, chloro[(4S)-2-[2-(diphenylphosphino-κP)phenyl]-4,5-dihydro-4-(1-methylethyl)oxazole-κN3]methyl-, (SP-4-2)-(9CI) (CA INDEX NAME)



CC 29-13 (Organometallic and Organometalloidal Compounds)
Section cross-reference(s): 23, 24, 67, 75
IT **Asymmetric synthesis and induction**
(in Michael reaction of α-cyano carboxylates with Me vinyl ketone catalyzed by organoplatinum (phosphinophenyl)oxazoline enantiomerically pure complexes)
IT **Michael reaction**
(stereoselective; of α-cyano carboxylates with Me vinyl ketone catalyzed by organoplatinum (phosphinophenyl)oxazoline complexes)
IT **Michael reaction catalysts**
(stereoselective; organoplatinum (phosphinophenyl)oxazoline complexes for reaction of α-cyano carboxylates with Me

vinyl ketone)
IT **78-94-4**, Methyl vinyl ketone, reactions
RL: RCT (Reactant); **RACT (Reactant or reagent)**
(asym. Michael reaction with Et cyanopropionate catalyzed by organoplatinum (phosphinophenyl)oxazoline complexes)
IT **239099-78-6P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and chlorination of)
IT **239099-80-0DP**, petroleum ether solvate
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and crystal structure of)
IT **239099-81-1P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction with dichloromethane and silver tetrafluoroborate)
IT **239099-83-3P**
RL: CAT (Catalyst use); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation as enantioselective Michael reaction catalysts for reaction of α-cyano carboxylates with Me vinyl ketone)
IT **239099-85-5P**
RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(preparation as enantioselective Michael reaction catalysts for reaction of α-cyano carboxylates with Me vinyl ketone)
IT 143619-24-3P **239099-87-7P** **239099-89-9P** **239099-91-3P** **239099-93-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
IT **239099-79-7P**
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation, crystal structure, and chlorination of)
IT **239099-80-0P**
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation, mol. structure, and reaction with dichloromethane and silver tetrafluoroborate)

REFERENCE COUNT: 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L93 ANSWER 23 OF 34 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1998:270307 HCAPLUS
DOCUMENT NUMBER: 129:67541
TITLE: A New Palladium(II)-Catalyzed Asymmetric Chlorohydrin Synthesis
AUTHOR(S): El-Qisairi, Arab; Hamed, Othman; Henry, Patrick M.
CORPORATE SOURCE: Department of Chemistry, Loyola University of Chicago, Chicago, IL, 60626, USA
SOURCE: Journal of Organic Chemistry (**1998**), 63(9), 2790-2791
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal

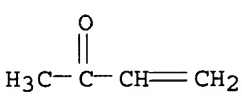
LANGUAGE: English
OTHER SOURCE(S): CASREACT 129:67541

AB Previous studies show that addition of a neutral ligand, L, to the coordination sphere of PdCl42- to give PdCl3L- under the conditions of the Wacker reaction changes the product from exclusively acetaldehyde to mainly 2-chloroethanol. Oxidation of α-olefins with a catalyst in which the neutral ligand is a chiral amine or phosphine should result in chiral chlorohydrins. Oxidation of propene with a catalyst containing a chiral amine produced propylene chlorohydrin with an optical purity of 10-15% ee. Catalysts containing chiral diphosphines should increase the optical purities. However, the neutral catalyst, PdCl2(L*-L*) is insol. in the reaction media. The solution to this problem involved two distinct approaches. The first approach used monometallic catalysts containing sulfonated p-Tol-BINAP ligands to increase solubility Optical purities ranged from 46% ee for propene to 76% ee for allyl Ph ether. The second approach used bimetallic catalysts containing a β-triketone and bridging chiral phosphine. Optical purities were higher for this system. The % ee's were >80% for all olefins tested. The highest were observed for propene with 94% ee and allyl Ph ether with 93% ee.

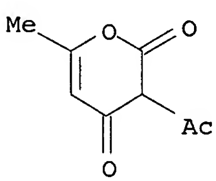
ED Entered STN: 13 May 1998

IT **78-94-4**, 3-Buten-2-one, reactions **520-45-6**, Dehydroacetic acid **14220-64-5**, Bis(benzonitrile)dichloropalladium
RL: RCT (Reactant); RACT (Reactant or reagent)
(palladium(II)-catalyzed asym. chlorohydrin synthesis)

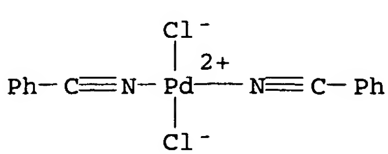
RN 78-94-4 HCAPLUS
CN 3-Buten-2-one (8CI, 9CI) (CA INDEX NAME)



RN 520-45-6 HCAPLUS
CN 2H-Pyran-2,4(3H)-dione, 3-acetyl-6-methyl- (8CI, 9CI) (CA INDEX NAME)



RN 14220-64-5 HCAPLUS
CN Palladium, bis(benzonitrile)dichloro- (8CI, 9CI) (CA INDEX NAME)



CC 25-7 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
Section cross-reference(s): 23

IT **Asymmetric synthesis and induction**
(palladium(II)-catalyzed asym. chlorohydrin synthesis)

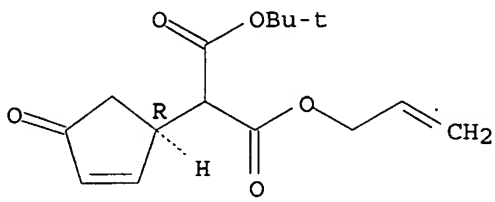
IT 75-05-8, Acetonitrile, reactions **78-94-4**, 3-Buten-2-one, reactions 90-15-3, 1-Naphthol 93-58-3, Methyl benzoate 106-95-6, Allyl bromide, reactions 109-67-1, 1-Pentene 115-07-1, 1-Propene, reactions 123-54-6, 2,4-Pentanedione, reactions **520-45-6**, Dehydroacetic acid 592-41-6, 1-Hexene, reactions 1746-13-0, Allyl phenyl ether 7440-05-3, Palladium, reactions 10025-98-6, Dipotassium tetrachloropalladate **14220-64-5**, Bis(benzonitrile)dichloropalladium 14635-75-7, Nitrosonium tetrafluoroborate 37676-25-8 76189-56-5, (S)-BINAP 86342-85-0 99646-28-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(palladium(II)-catalyzed asym. chlorohydrin synthesis)

REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L93 ANSWER 24 OF 34 HCAPLUS COPYRIGHT 2006 ACS on STN

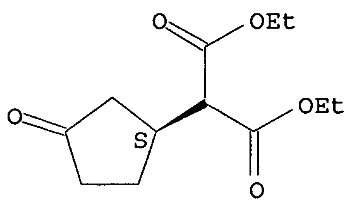
ACCESSION NUMBER:	1997:474075 HCAPLUS
DOCUMENT NUMBER:	127:161626
TITLE:	Asymmetric total syntheses of (+)-coronafacic acid and (+)-coronatine, phytotoxins isolated from Pseudomonas syringae pathovars
AUTHOR(S):	Nara, Shinji; Toshima, Hiroaki; Ichihara, Akitami
CORPORATE SOURCE:	Department Bioscience Chemistry, Faculty Agriculture, Hokkaido University, Sapporo, 060, Japan
SOURCE:	Tetrahedron (**1997**), 53(28), 9509-9524 CODEN: TETRAB; ISSN: 0040-4020
PUBLISHER:	Elsevier
DOCUMENT TYPE:	Journal
LANGUAGE:	English
OTHER SOURCE(S):	CASREACT 127:161626

GI



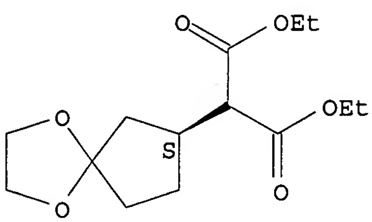
RN 193530-87-9 HCAPLUS
CN Propanedioic acid, [(1S)-3-oxocyclopentyl]-, diethyl ester (9CI)
(CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

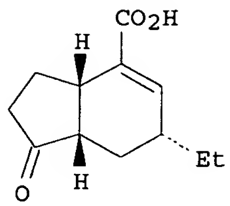


RN 193530-88-0 HCAPLUS
CN Propanedioic acid, (7S)-1,4-dioxaspiro[4.4]non-7-yl-, diethyl
ester (9CI) (CA INDEX NAME)

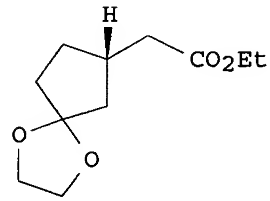
Absolute stereochemistry. Rotation (+).



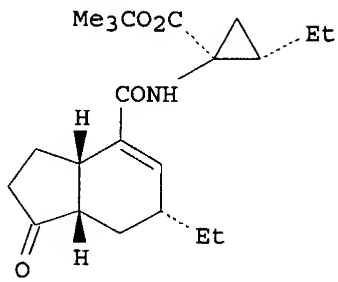
CC 26-9 (Biomolecules and Their Synthetic Analogs)
IT **Asymmetric synthesis and induction**
(asym. total syntheses of (+)-coronafacic acid and
(+)-coronatine)
IT 105-53-3, Diethyl malonate 922-63-4, 2-Ethylacrolein
930-30-3, 2-Cyclopentenone 59995-48-1 62457-60-7
166826-51-3 183253-55-6
RL: RCT (Reactant); **RACT (Reactant or reagent)**
(asym. total syntheses of (+)-coronafacic acid and
(+)-coronatine)
IT 42726-73-8P 79405-48-4P 93306-08-2P 132665-05-5P
134209-82-8P 183115-24-4P 183115-27-7P 189506-59-0P
189506-61-4P 190073-22-4P 193530-85-7P **193530-86-8P**
193530-87-9P 193530-88-0P 193530-90-4P
193530-91-5P 193530-92-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP
(Preparation); RACT (Reactant or reagent)
(asym. total syntheses of (+)-coronafacic acid and
(+)-coronatine)



I



II



III

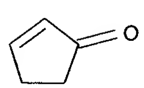
AB Asym. total synthesis of (+)-coronafacic acid (I), was accomplished via intramol. 1,6-conjugate addition as the key step. The chiral ester (+)-II was prepared via two approaches: starting from (R)-(+)-4-acetoxy-2-cyclopenten-1-one, and using catalytic asym. Michael reactions promoted by heterobimetallic BINOL complexes. Coupling between (+)-I and the protected coronamic acid and subsequent deprotection by hydrogenolysis provided (+)-coronatine (III). This is the first asym. total synthesis of (+)-III.

ED Entered STN: 30 Jul 1997

IT **930-30-3**, 2-Cyclopentenone
RL: RCT (Reactant); **RACT (Reactant or reagent)**
(asym. total syntheses of (+)-coronafacic acid and (+)-coronatine)

RN 930-30-3 HCAPLUS

CN 2-Cyclopenten-1-one (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



IT **193530-86-8P 193530-87-9P 193530-88-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(asym. total syntheses of (+)-coronafacic acid and (+)-coronatine)

RN 193530-86-8 HCAPLUS

CN Propanedioic acid, (4-oxo-2-cyclopenten-1-yl)-, 1,1-dimethylethyl 2-propenyl ester, (1R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

REFERENCE COUNT: 40 THERE ARE 40 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L93 ANSWER 25 OF 34 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1996:513724 HCAPLUS
DOCUMENT NUMBER: 125:220828
TITLE: Michael Reaction of Stabilized Carbon Nucleophiles Catalyzed by [RuH2(PPh3)4]
AUTHOR(S): Gomez-Bengoa, Enrique; Cuerva, Juan M.; Mateo, Cristina; Echavarren, Antonio M.
CORPORATE SOURCE: Departamento de Quimica Organica, Universidad Autonoma de Madrid, Madrid, 28049, Spain
SOURCE: Journal of the American Chemical Society (**1996**), 118(36), 8553-8565
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 125:220828

AB The Michael reaction of active methylene compds. lacking cyano groups such as malonates, β-ketoesters, 1,3-diketones, 1,1-disulfones, nitro compds., Meldrum acid, and anthrone with common acceptors proceeds in acetonitrile solution in the presence of [RuH2(PPh3)4] as the catalyst. Cyano acetates, more acidic than malonates in organic solvents, are also excellent substrates for this reaction. In a number of cases, intramol. aldol reactions catalyzed by [RuH2(PPh3)4] were also observed as side reactions. Catalysis by other ruthenium and rhodium complexes has been examined Selectivity studies performed with malonate and disulfone donors indicate that the catalyst selectively activates Michael donors that can coordinate with ruthenium(II). Addnl., it has been shown that the reaction requires the presence of free phosphine. Therefore, the Michael reaction of stabilized enolates appears to be a ruthenium- and phosphine-catalyzed reaction. From a practical point of view, the use of readily prepared [RuH2(PPh3)4] as the catalyst in acetonitrile provided the best solution for the Michael reaction of active methylene compds.

ED Entered STN: 28 Aug 1996

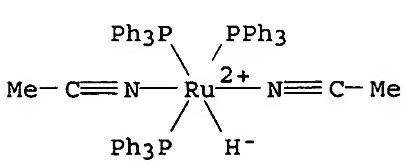
IT **40988-90-7 132751-57-6**
RL: CAT (Catalyst use); USES (Uses)
(Michael reaction of stabilized carbon nucleophiles catalyzed by [RuH2(PPh3)4] and related compds.)

RN 40988-90-7 HCAPLUS

CN Ruthenium(1+), bis(acetonitrile)hydrotris(triphenylphosphine)-, (OC-6-21)-, hexafluorophosphate(1-) (9CI) (CA INDEX NAME)

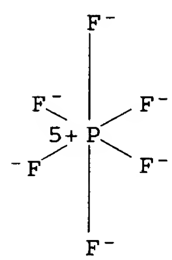
CM 1

CRN 48245-15-4
CMF C58 H52 N2 P3 Ru
CCI CCS



CM 2

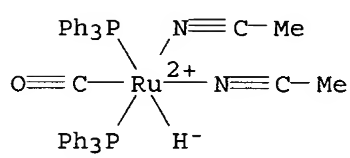
CRN 16919-18-9
CMF F6 P
CCI CCS



RN 132751-57-6 HCAPLUS
CN Ruthenium(1+), bis(acetonitrile)carbonylhydrobis(triphenylphosphin
e)-, (OC-6-14)-, tetrafluoroborate(1-) (9CI) (CA INDEX NAME)

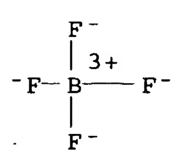
CM 1

CRN 47868-22-4
CMF C41 H37 N2 O P2 Ru
CCI CCS

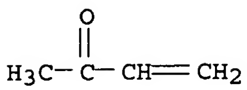


CM 2

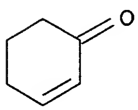
CRN 14874-70-5
CMF B F4
CCI CCS



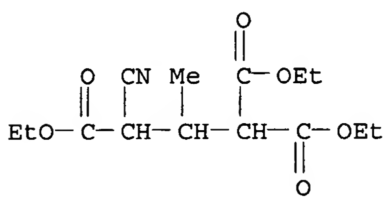
IT **78-94-4**, Methyl vinyl ketone, reactions **930-68-7**
, 2-Cyclohexen-1-one **121730-78-7**
RL: RCT (Reactant); RACT (Reactant or reagent)
(Michael reaction of stabilized carbon nucleophiles catalyzed
by [RuH2(PPh3)4] and related compds.)
RN 78-94-4 HCAPLUS
CN 3-Buten-2-one (8CI, 9CI) (CA INDEX NAME)



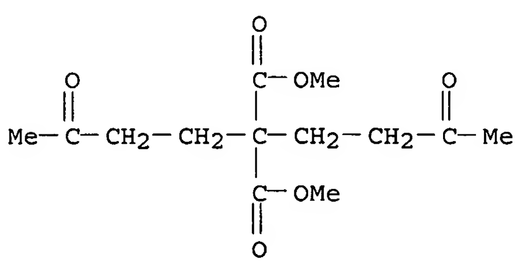
RN 930-68-7 HCAPLUS
CN 2-Cyclohexen-1-one (6CI, 8CI, 9CI) (CA INDEX NAME)



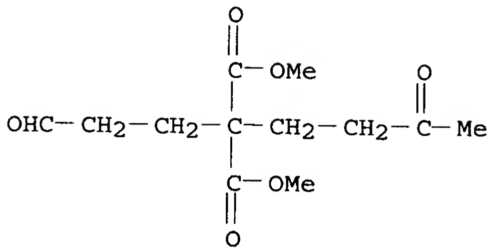
RN 121730-78-7 HCAPLUS
CN 1,1,3-Propanetricarboxylic acid, 3-cyano-2-methyl-, triethyl ester (9CI) (CA INDEX NAME)



IT **151920-47-7P 181186-01-6P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(Michael reaction of stabilized carbon nucleophiles catalyzed by [RuH2(PPh3)4] and related compds.)
RN 151920-47-7 HCAPLUS
CN Propanedioic acid, bis(3-oxobutyl)-, dimethyl ester (9CI) (CA INDEX NAME)



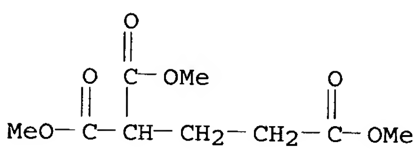
RN 181186-01-6 HCAPLUS
CN Propanedioic acid, (3-oxobutyl)(3-oxopropyl)-, dimethyl ester (9CI) (CA INDEX NAME)



IT 1733-16-0P 25112-78-1P 33646-18-3P
42593-60-2P 59104-44-8P 95929-65-0P
181185-88-6P 181185-89-7P 181185-90-0P
181185-92-2P 181185-93-3P 181185-94-4P
181185-95-5P 181185-96-6P 181186-02-7P
181186-03-8P 181186-04-9P 181186-05-0P
181186-06-1P 181377-47-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(Michael reaction of stabilized carbon nucleophiles catalyzed by [RuH2(PPh3)4] and related compds.)

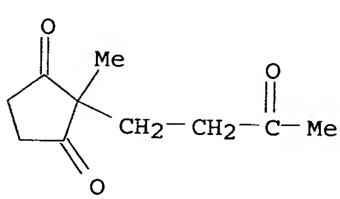
RN 1733-16-0 HCAPLUS

CN 1,1,3-Propanetricarboxylic acid, trimethyl ester (7CI, 8CI, 9CI) (CA INDEX NAME)



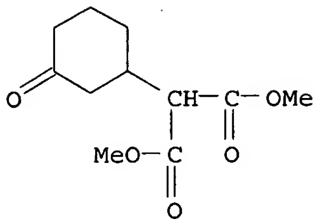
RN 25112-78-1 HCAPLUS

CN 1,3-Cyclopentanedione, 2-methyl-2-(3-oxobutyl)- (6CI, 8CI, 9CI) (CA INDEX NAME)

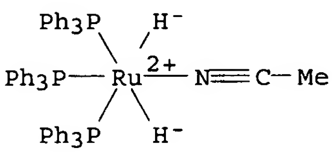


RN 33646-18-3 HCAPLUS

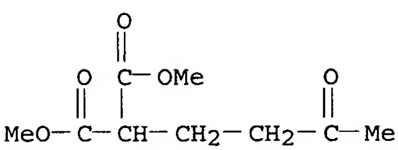
CN Propanedioic acid, (3-oxocyclohexyl)-, dimethyl ester (9CI) (CA INDEX NAME)



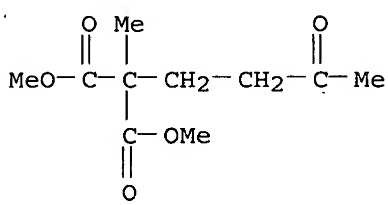
RN 42593-60-2 HCAPLUS
CN Ruthenium, (acetonitrile)dihydrotris(triphenylphosphine)- (9CI) (CA INDEX NAME)



RN 59104-44-8 HCAPLUS
CN Propanedioic acid, (3-oxobutyl)-, dimethyl ester (9CI) (CA INDEX NAME)

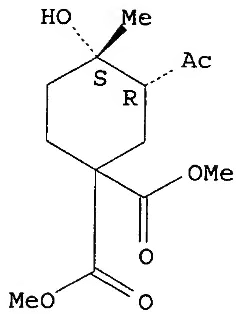


RN 95929-65-0 HCAPLUS
CN Propanedioic acid, methyl(3-oxobutyl)-, dimethyl ester (9CI) (CA INDEX NAME)

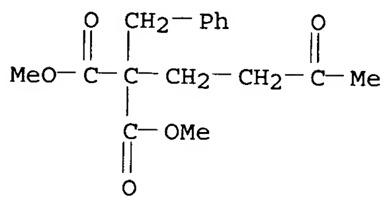


RN 181185-88-6 HCAPLUS
CN 1,1-Cyclohexanedicarboxylic acid, 3-acetyl-4-hydroxy-4-methyl-, dimethyl ester, cis- (9CI) (CA INDEX NAME)

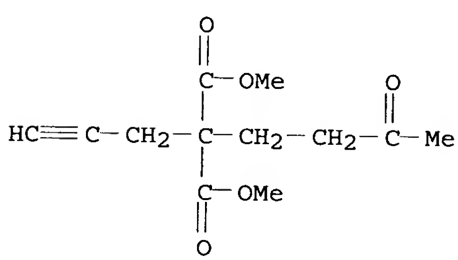
Relative stereochemistry.



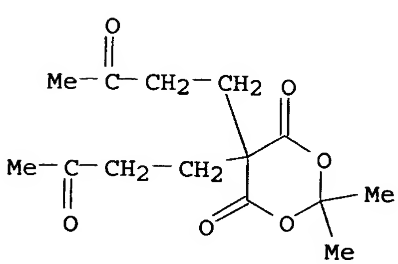
RN 181185-89-7 HCAPLUS
CN Propanedioic acid, (3-oxobutyl)(phenylmethyl)-, dimethyl ester
(9CI) (CA INDEX NAME)



RN 181185-90-0 HCAPLUS
CN Propanedioic acid, (3-oxobutyl)-2-propynyl-, dimethyl ester (9CI)
(CA INDEX NAME)

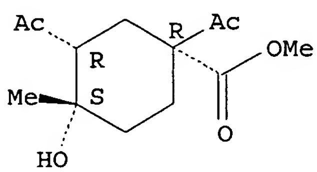


RN 181185-92-2 HCAPLUS
CN 1,3-Dioxane-4,6-dione, 2,2-dimethyl-5,5-bis(3-oxobutyl)- (9CI)
(CA INDEX NAME)

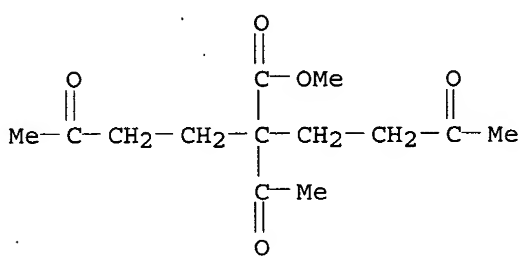


RN 181185-93-3 HCAPLUS
CN Cyclohexanecarboxylic acid, 1,3-diacetyl-4-hydroxy-4-methyl-, methyl ester, (1α,3α,4α)- (9CI) (CA INDEX NAME)

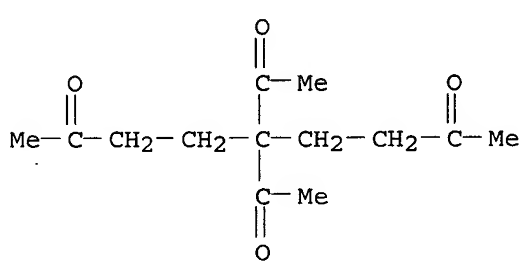
Relative stereochemistry.



RN 181185-94-4 HCAPLUS
CN Hexanoic acid, 2-acetyl-5-oxo-2-(3-oxobutyl)-, methyl ester (9CI) (CA INDEX NAME)

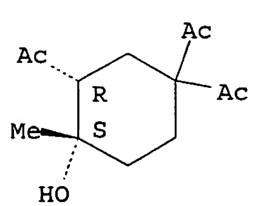


RN 181185-95-5 HCAPLUS
CN 2,8-Nonanedione, 5,5-diacetyl- (9CI) (CA INDEX NAME)



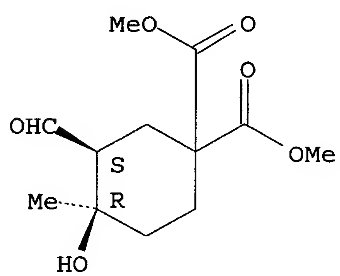
RN 181185-96-6 HCAPLUS
CN Ethanone, 1,1',1''-[(1R,6S)-6-hydroxy-6-methyl-1-cyclohexanyl-3-ylidene]tris-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



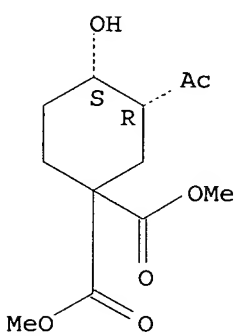
RN 181186-02-7 HCAPLUS
CN 1,1-Cyclohexanedicarboxylic acid, 3-formyl-4-hydroxy-4-methyl-, dimethyl ester, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



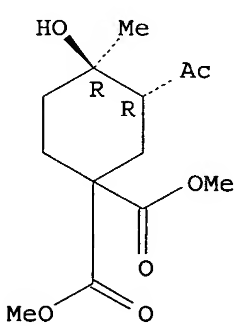
RN 181186-03-8 HCAPLUS
CN 1,1-Cyclohexanedicarboxylic acid, 3-acetyl-4-hydroxy-, dimethyl ester, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



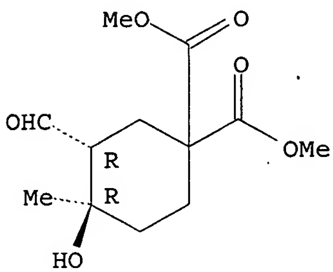
RN 181186-04-9 HCAPLUS
CN 1,1-Cyclohexanedicarboxylic acid, 3-acetyl-4-hydroxy-4-methyl-, dimethyl ester, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



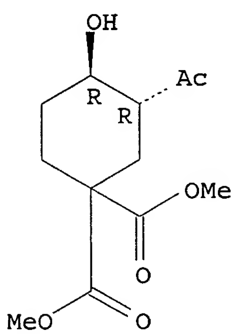
RN 181186-05-0 HCAPLUS
CN 1,1-Cyclohexanedicarboxylic acid, 3-formyl-4-hydroxy-4-methyl-, dimethyl ester, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



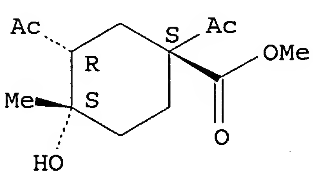
RN 181186-06-1 HCAPLUS
CN 1,1-Cyclohexanedicarboxylic acid, 3-acetyl-4-hydroxy-, dimethyl ester, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 181377-47-9 HCAPLUS
CN Cyclohexanecarboxylic acid, 1,3-diacetyl-4-hydroxy-4-methyl-, methyl ester, (1α,3β,4β)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



CC 21-2 (General Organic Chemistry)
IT **Michael reaction**
Michael reaction catalysts
(Michael reaction of stabilized carbon nucleophiles catalyzed by [RuH2(PPh3)4] and related compds.)
IT 603-32-7, Triphenylarsine 603-35-0, Triphenylphosphine, uses 998-40-3, Tributylphosphine 2622-14-2, Tricyclohexylphosphine 12150-46-8, Dppf 15529-49-4 22172-51-6 22337-78-6 **40988-90-7** 61521-25-3 74735-07-2 114595-94-7 132724-29-9 **132751-57-6** 156734-49-5 157931-51-6 181377-46-8

RL: CAT (Catalyst use); USES (Uses)
(Michael reaction of stabilized carbon nucleophiles catalyzed by [RuH2(PPh3)4] and related compds.)

IT **78-94-4**, Methyl vinyl ketone, reactions 79-24-3, Nitroethane 86-73-7, Fluorene 90-44-8, Anthrone 96-33-3, Methyl acrylate 105-45-3, Methyl 3-oxobutyrate 105-56-6, Ethyl cyanoacetate 107-02-8, 2-Propenal, reactions 107-13-1, 2-Propenenitrile, reactions 108-59-8, Dimethyl malonate 123-54-6, 2,4-Pentanedione, reactions 538-58-9, Dibenzylideneacetone 609-02-9, Dimethyl methylmalonate 624-49-7, Dimethyl fumarate 765-69-5 **930-68-7**, 2-Cyclohexen-1-one 2033-24-1 3406-02-8, Bis(phenylsulfonyl)methane 4170-30-3, Crotonaldehyde 5535-48-8, Phenyl vinyl sulfone 49769-78-0, Dimethyl benzylmalonate 50765-99-6 54083-06-6 95124-07-5 **121730-78-7** 133817-97-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(Michael reaction of stabilized carbon nucleophiles catalyzed by [RuH2(PPh3)4] and related compds.)

IT 72473-15-5P **151920-47-7P** **181186-01-6P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(Michael reaction of stabilized carbon nucleophiles catalyzed by [RuH2(PPh3)4] and related compds.)

IT **1733-16-0P** 19766-36-0P **25112-78-1P** **33646-18-3P** 35223-72-4P **42593-60-2P** 55525-27-4P **59104-44-8P** 81794-16-3P 87625-87-4P **95929-65-0P** 136917-89-0P 173593-86-7P **181185-88-6P** **181185-89-7P** **181185-90-0P** 181185-91-1P **181185-92-2P** **181185-93-3P** **181185-94-4P** **181185-95-5P** **181185-96-6P** 181185-97-7P 181185-98-8P 181185-99-9P 181186-00-5P **181186-02-7P** **181186-03-8P** **181186-04-9P** **181186-05-0P** **181186-06-1P** 181186-07-2P 181186-08-3P 181186-09-4P 181186-10-7P 181186-11-8P 181186-14-1P 181377-43-5P **181377-47-9P** 181377-48-0P 181377-49-1P 181377-50-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(Michael reaction of stabilized carbon nucleophiles catalyzed by [RuH2(PPh3)4] and related compds.)

L93 ANSWER 26 OF 34 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1996:380129 HCAPLUS
DOCUMENT NUMBER: 125:86908
TITLE: A New Catalyst for a Pd Catalyzed Alder Ene Reaction. A Total Synthesis of (+)-Cassiol
AUTHOR(S): Trost, Barry M.; Li, Yong
CORPORATE SOURCE: Department of Chemistry, Stanford University, Stanford, CA, 94305, USA
SOURCE: Journal of the American Chemical Society (**1996**), 118(28), 6625-6633
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 125:86908
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

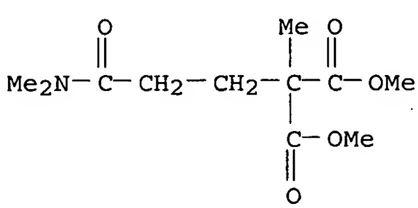
AB The scope of the palladium catalyzed cycloisomerization of enynes, e.g. alkyne I to cyclohexanone II, in an Alder ene type fashion that led to a new catalytic system was explored in the context of a synthetic strategy to the antiulcerogenic agent (+)-cassiol (III). In a model study, the effect of six-membered ring formation, the presence of a carbonyl group in the tether, and the steric hindrance of the alkene conspire to prevent the cycloisomerization under the "standard" conditions. Two variables proved key in the development of a new catalytic system that has proven to be effective, the absence of traditional ligands and the choice of acid. An effective synthesis of (+)-cassiol (III) was accomplished in which this new reaction played a key. A lipase served to introduce the chirality, and a palladium(0) catalyzed reaction was important in elaborating a side chain. The final adjustment of oxidation level made advantageous use of a platinum catalyzed enone hydrosilyation.

ED Entered STN: 02 Jul 1996

IT **178559-14-3P**
RL: BPR (Biological process); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); PROC (Process); RACT (Reactant or reagent)
(total synthesis of(+)-cassiol via palladium-catalyzed Alder ene reaction)

RN 178559-14-3 HCAPLUS

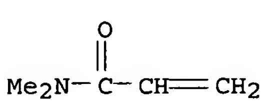
CN Propanedioic acid, [3-(dimethylamino)-3-oxopropyl]methyl-, dimethyl ester (9CI) (CA INDEX NAME)



IT **2680-03-7**
RL: RCT (Reactant); **RACT (Reactant or reagent)**
(total synthesis of(+)-cassiol via palladium-catalyzed Alder ene reaction)

RN 2680-03-7 HCAPLUS

CN 2-Propenamide, N,N-dimethyl- (9CI) (CA INDEX NAME)



CC 30-15 (Terpenes and Terpenoids)
Section cross-reference(s): 26, 33

IT **Asymmetric synthesis and induction**
(total synthesis of(+)-cassiol via palladium-catalyzed Alder ene reaction)

IT 178559-14-3P
RL: BPR (Biological process); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); PROC (Process); RACT (Reactant or reagent)
(total synthesis of(+)-cassiol via palladium-catalyzed Alder ene reaction)

IT 108-59-8, Dimethyl malonate 609-02-9, Dimethyl methylmalonate 1066-54-2, (Trimethylsilyl)acetylene **2680-03-7** 5497-67-6, 2,2-Dimethyl-4-pentenal
RL: RCT (Reactant); **RACT (Reactant or reagent)**
(total synthesis of(+)-cassiol via palladium-catalyzed Alder ene reaction)

L93 ANSWER 27 OF 34 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1996:259869 HCAPLUS
DOCUMENT NUMBER: 125:32888
TITLE: Asymmetric Michael Addition of Malonate Anions to Prochiral Acceptors Catalyzed by L-Proline Rubidium Salt
AUTHOR(S): Yamaguchi, Masahiko; Shiraishi, Tai; Hirama, Masahiro
CORPORATE SOURCE: Graduate School of Science, Tohoku University, Sendai, 980-77, Japan
SOURCE: Journal of Organic Chemistry (**1996**), 61(10), 3520-30
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 125:32888

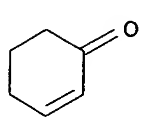
AB L-Proline rubidium salt catalyzes the asym. Michael addition of malonate anions to prochiral enones and enals. This method can be applied to a wide range of substrates to give adducts with a predictable absolute configuration: (S)-adducts from (E)-enones/enals and (R)-adducts from cyclic (Z)-enones. Both the secondary amine moiety and the carboxylate moiety are critical for the catalytic activity and asym. induction. Varying the countercation also affects the reaction course. High enantiomeric excesses were attained when di-tert-Bu malonate was added to (E)-enones in the presence of CsF. The stereochem. of the Michael reaction indicates that asym. induction takes place via enantioface discrimination involving the acceptor α-carbon atom rather than the β-carbon atom.

ED Entered STN: 03 May 1996

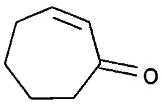
IT **930-68-7**, 2-Cyclohexenone **1121-66-0**, 2-Cycloheptenone **3102-33-8 32397-56-1 50396-87-7**
RL: RCT (Reactant); **RACT (Reactant or reagent)**
(asym. Michael addition of malonate anions to prochiral acceptors catalyzed by L-proline rubidium salt)

RN 930-68-7 HCAPLUS

CN 2-Cyclohexen-1-one (6CI, 8CI, 9CI) (CA INDEX NAME)

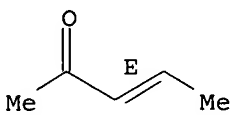


RN 1121-66-0 HCAPLUS
CN 2-Cyclohepten-1-one (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



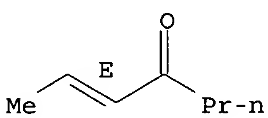
RN 3102-33-8 HCAPLUS
CN 3-Penten-2-one, (3E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



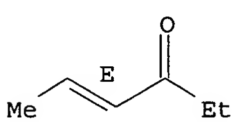
RN 32397-56-1 HCAPLUS
CN 2-Hepten-4-one, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



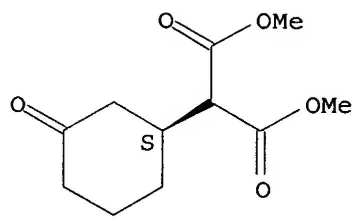
RN 50396-87-7 HCAPLUS
CN 4-Hexen-3-one, (4E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

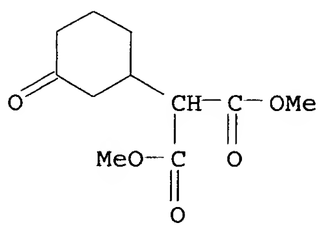


IT **154194-50-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(asym. Michael addition of malonate anions to prochiral acceptors catalyzed by L-proline rubidium salt)
RN 154194-50-0 HCAPLUS
CN Propanedioic acid, [(1S)-3-oxocyclohexyl]-, dimethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

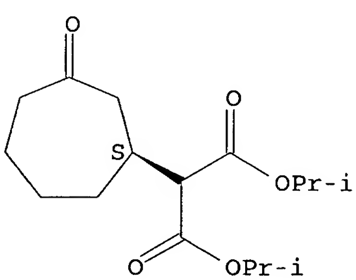


IT 33646-18-3P 177722-12-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(asym. Michael addition of malonate anions to prochiral acceptors catalyzed by L-proline rubidium salt)
RN 33646-18-3 HCAPLUS
CN Propanedioic acid, (3-oxocyclohexyl)-, dimethyl ester (9CI) (CA INDEX NAME)



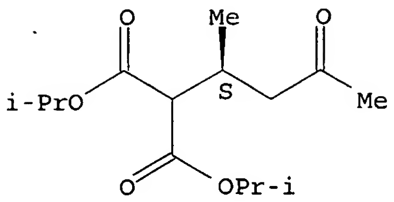
RN 177722-12-2 HCAPLUS
CN Propanedioic acid, (3-oxocycloheptyl)-, bis(1-methylethyl) ester, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



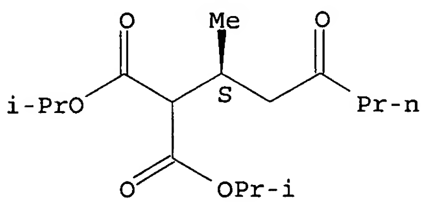
IT **151600-45-2P 151600-46-3P 164931-77-5P 164931-78-6P 177722-13-3P 177722-18-8P 177722-20-2P 177722-22-4P 177722-26-8P 177722-27-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 151600-45-2 HCAPLUS
CN Propanedioic acid, (1-methyl-3-oxobutyl)-, bis(1-methylethyl) ester, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



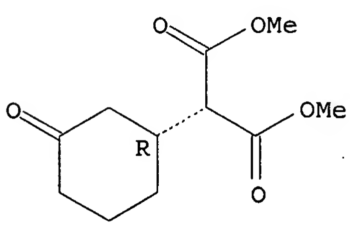
RN 151600-46-3 HCAPLUS
CN Propanedioic acid, (1-methyl-3-oxohexyl)-, bis(1-methylethyl)
ester, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



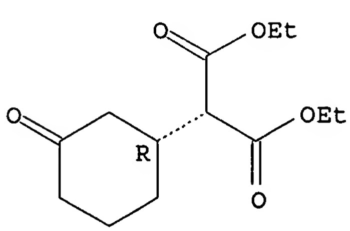
RN 164931-77-5 HCAPLUS
CN Propanedioic acid, [(1R)-3-oxocyclohexyl]-, dimethyl ester (9CI)
(CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



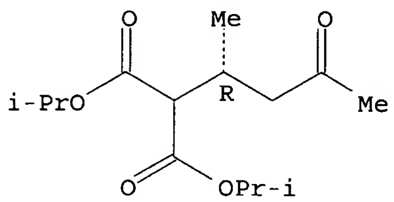
RN 164931-78-6 HCAPLUS
CN Propanedioic acid, [(1R)-3-oxocyclohexyl]-, diethyl ester (9CI)
(CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



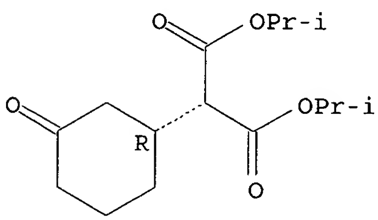
RN 177722-13-3 HCAPLUS
CN Propanedioic acid, (1-methyl-3-oxobutyl)-, bis(1-methylethyl)
ester, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



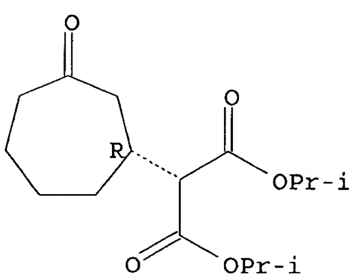
RN 177722-18-8 HCAPLUS
CN Propanedioic acid, [(1R)-3-oxocyclohexyl]-, bis(1-methylethyl) ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



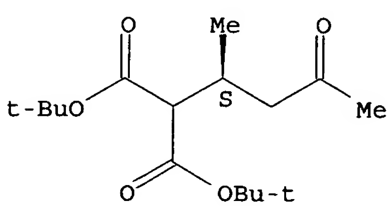
RN 177722-20-2 HCAPLUS
CN Propanedioic acid, (3-oxocycloheptyl)-, bis(1-methylethyl) ester, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



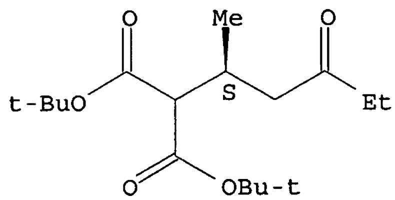
RN 177722-22-4 HCAPLUS
CN Propanedioic acid, [(1S)-1-methyl-3-oxobutyl]-, bis(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



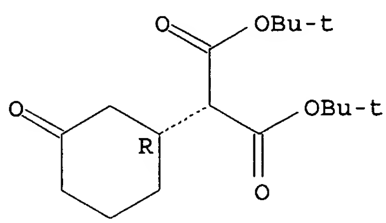
RN 177722-26-8 HCAPLUS
CN Propanedioic acid, (1-methyl-3-oxopentyl)-, bis(1,1-dimethylethyl) ester, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 177722-27-9 HCAPLUS
CN Propanedioic acid, [(1R)-3-oxocyclohexyl]-, bis(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



CC 21-2 (General Organic Chemistry)
IT **Asymmetric synthesis and induction**
Michael reaction
(asym. Michael addition of malonate anions to prochiral acceptors catalyzed by L-proline rubidium salt)
IT **Michael reaction catalysts**
RL: CAT (Catalyst use); USES (Uses)
(asym. Michael addition of malonate anions to prochiral acceptors catalyzed by L-proline rubidium salt)
IT 79-46-9, 2-Nitropropane 105-53-3, Diethyl malonate 108-59-8, Dimethyl malonate 110-52-1, 1,4-Dibromobutane 123-73-9 541-16-2, Di-tert-butyl malonate 627-05-4, 1-Nitrobutane **930-68-7**, 2-Cyclohexenone **1121-66-0**, 2-Cycloheptenone 1694-31-1, tert-Butyl acetoacetate 1896-62-4 **3102-33-8** 6221-50-7 6728-26-3 13195-64-7, Diisopropyl malonate 15014-25-2, Dibenzyl malonate 18402-83-0 23356-96-9, L-Prolinol 25112-78-1 **32397-56-1** **50396-87-7** 56161-62-7 56345-01-8, (E)-2-Cyclopentadecenone
RL: RCT (Reactant); **RACT (Reactant or reagent)**
(asym. Michael addition of malonate anions to prochiral acceptors catalyzed by L-proline rubidium salt)
IT 33879-04-8P 84308-30-5P 151600-48-5P **154194-50-0P** 177722-17-7P 177770-85-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(asym. Michael addition of malonate anions to prochiral acceptors catalyzed by L-proline rubidium salt)
IT **33646-18-3P** 63975-98-4P, (S)-(+)-Muscone 108329-93-7P

177722-12-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(asym. Michael addition of malonate anions to prochiral acceptors catalyzed by L-proline rubidium salt)

IT 17553-86-5P 89393-67-9P 96634-75-2P 108056-65-1P **151600-45-2P** **151600-46-3P** 151600-47-4P 151600-51-0P 160012-11-3P 160012-12-4P 160012-13-5P 160012-14-6P 160622-04-8P 160632-29-1P 164931-75-3P **164931-77-5P** **164931-78-6P** **177722-13-3P** 177722-14-4P 177722-15-5P 177722-16-6P **177722-18-8P** 177722-19-9P **177722-20-2P** 177722-21-3P **177722-22-4P** 177722-23-5P 177722-24-6P 177722-25-7P **177722-26-8P** **177722-27-9P** 177722-28-0P 177722-29-1P 177722-30-4P 177722-31-5P 177770-89-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

L93 ANSWER 28 OF 34 HCAPLUS COPYRIGHT 2006 ACS on STN

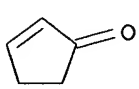
ACCESSION NUMBER:	1996:71012 HCAPLUS
DOCUMENT NUMBER:	124:231881
TITLE:	A new multifunctional heterobimetallic asymmetric catalyst for Michael additions and tandem Michael-aldol reactions
AUTHOR(S):	Arai, Takayoshi; Sasai, Hiroaki; Aoe, Kei-ichi; Okamura, Kimio; Date, Tadamasa; Shibasaki, Masakatsu
CORPORATE SOURCE:	Fac. Pharmaceutical Sci., Univ. Tokyo, Tokyo, 113, Japan
SOURCE:	Angewandte Chemie, International Edition in English (**1996**), 35(1), 104-6 CODEN: ACIEAY; ISSN: 0570-0833
PUBLISHER:	VCH
DOCUMENT TYPE:	Journal
LANGUAGE:	English
OTHER SOURCE(S):	CASREACT 124:231881

AB AlLi-BINOL complex was prepared from (R)-BINOL, diisobutylaluminum hydride, and BuLi and examined as a catalyst for Michael and Michael-aldol reactions of 2-cyclopentenone and 2-cyclohexenone. The structure of the product obtained from AlLi-BINOL and 2-cyclohexenone was determined by X-ray anal.

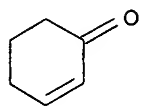
ED Entered STN: 01 Feb 1996

IT **930-30-3**, 2-Cyclopentenone **930-68-7**, 2-Cyclohexenone
RL: RCT (Reactant); **RACT (Reactant or reagent)**
(aluminum-BINOL complex as asym. catalyst for Michael addns. and tandem Michael-aldol reactions)

RN 930-30-3 HCAPLUS
CN 2-Cyclopenten-1-one (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

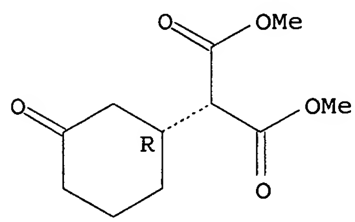


RN 930-68-7 HCAPLUS
CN 2-Cyclohexen-1-one (6CI, 8CI, 9CI) (CA INDEX NAME)



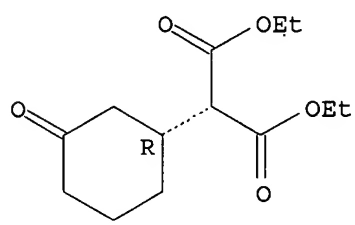
IT 164931-77-5P 164931-78-6P 174782-76-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(aluminum-BINOL complex as asym. catalyst for Michael addns. and tandem Michael-aldol reactions)
RN 164931-77-5 HCAPLUS
CN Propanedioic acid, [(1R)-3-oxocyclohexyl]-, dimethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



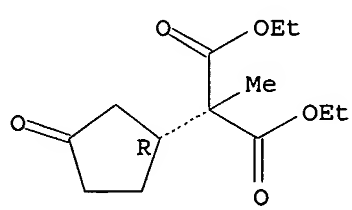
RN 164931-78-6 HCAPLUS
CN Propanedioic acid, [(1R)-3-oxocyclohexyl]-, diethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



RN 174782-76-4 HCAPLUS
CN Propanedioic acid, methyl[(1R)-3-oxocyclopentyl]-, diethyl ester (9CI) (CA INDEX NAME)

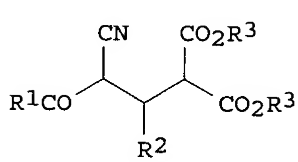
Absolute stereochemistry.



CC 24-5 (Alicyclic Compounds)
Section cross-reference(s): 75

IT Aldol condensation catalysts
Asymmetric synthesis and induction
Michael reaction catalysts
(aluminum-BINOL complex as asym. catalyst for Michael addns. and tandem Michael-aldol reactions)
IT 100-52-7, Benzaldehyde, reactions 104-53-0, 3-Phenylpropanal 105-53-3, Diethyl malonate 108-59-8, Dimethyl malonate 609-08-5, Diethyl methylmalonate **930-30-3**, 2-Cyclopentenone **930-68-7**, 2-Cyclohexenone 15014-25-2, Dibenzyl malonate
RL: RCT (Reactant); **RACT (Reactant or reagent)**
(aluminum-BINOL complex as asym. catalyst for Michael addns. and tandem Michael-aldol reactions)
IT 164931-75-3P **164931-77-5P 164931-78-6P**
174782-76-4P 174782-78-6P 174782-84-4P 185760-71-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(aluminum-BINOL complex as asym. catalyst for Michael addns. and tandem Michael-aldol reactions)

L93 ANSWER 29 OF 34 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1995:961627 HCAPLUS
DOCUMENT NUMBER: 124:174937
TITLE: Ruthenium-catalyzed aldol and Michael reactions of nitriles. Carbon-carbon bond formation by α-C-H activation of nitriles.
AUTHOR(S): Murahashi, Shun-Ichi; Naota, Takeshi; Taki, Hiroshi; Mizuno, Masahiko; Takaya, Hikaru; Komiya, Sanshiro; Mizuho, Yuji; Oyasato, Naohiko; Hiraoka, Makiko; et al.
CORPORATE SOURCE: Faculty of Engineering Science, Osaka University, Toyonaka, 560, Japan
SOURCE: Journal of the American Chemical Society (**1995**), 117(50), 12436-51
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 124:174937
GI



I

AB Ru(II)-catalyzed reaction of nitriles with carbonyl compds. proceeds efficiently under mild conditions to give α,β-unsatd. nitriles. Under similar reaction conditions, nitriles react with olefins bearing electron-withdrawing groups to give Michael adducts. The utility of the reaction is illustrated by selective addns. to α,β-unsatd. aldehydes and acetylenes bearing electron-withdrawing groups, which are difficult to perform using conventional bases. Chemoselective aldol and Michael reactions of nitriles can be performed in the presence of other active

methylene compds. Michael and tandem Michael-aldol condensations of nitriles (I; R1 = OMe, OEt, OBu, NH2; R2, R3 = Me, Et) with H2C:CHEWG (EWG = COMe, CN, COPh) can be performed with high diastereoselectivity. These reactions can be rationalized by assuming oxidative addition of Ru(0) to the α-C-H bond of nitriles and subsequent insertions to carbonyl compds. or olefins. As the key intermediates and active catalysts hydrido(N-bonded enolato)Ru(II) complexes, mer-RuH(NCCHCO2R)(NCCH2CO2R)(PPh3)3 (R = Me, Et, Bu) have been isolated upon treatment of RuH2(PPh3)4 or RuH(C2H4)(PPh3)2(PPh2C6H4) with alkyl cyanoacetates. Kinetic study of the catalytic aldol reaction of Et cyanoacetate with PhCHO indicates that the rate-determining step is the reaction of enolato complex with aldehydes.

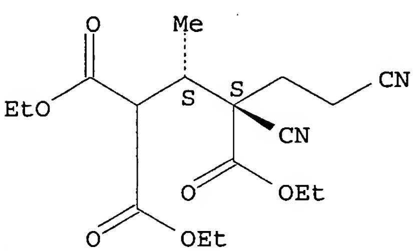
ED Entered STN: 05 Dec 1995

IT **173593-92-5P**
RL: BYP (Byproduct); PREP (Preparation)
(ruthenium-catalyzed aldol and Michael reactions of nitriles)

RN 173593-92-5 HCAPLUS

CN 1,1,3-Pentanetricarboxylic acid, 3,5-dicyano-2-methyl-, triethyl ester, (R*,R*)- (9CI) (CA INDEX NAME)

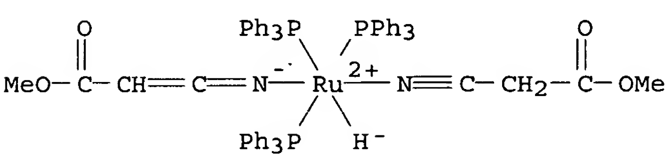
Relative stereochemistry.



IT **138614-12-7P 138614-14-9P**
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(ruthenium-catalyzed aldol and Michael reactions of nitriles)

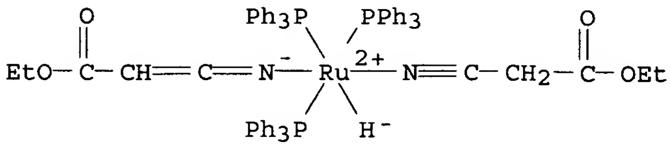
RN 138614-12-7 HCAPLUS

CN Ruthenium, hydro(methyl carbonimidoylacetato-N)(methyl cyanoacetate-N)tris(triphenylphosphine)-, (OC-6-31)- (9CI) (CA INDEX NAME)

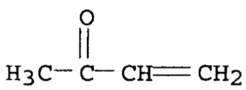


RN 138614-14-9 HCAPLUS

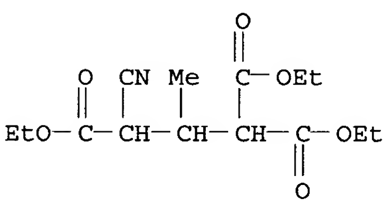
CN Ruthenium, [ethyl (cyano-κN)acetate][ethyl 3-(imino-κN)-2-propenoato]hydrotris(triphenylphosphine)-, (OC-6-31)- (9CI) (CA INDEX NAME)



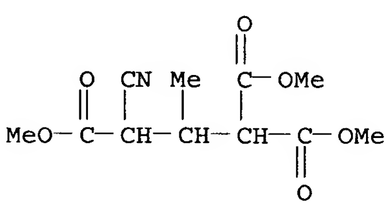
IT **78-94-4**, Methyl vinyl ketone, reactions
121730-78-7 **173594-02-0** **173594-03-1**
173594-04-2 **173594-05-3**
RL: RCT (Reactant); RACT (Reactant or reagent)
(ruthenium-catalyzed aldol and Michael reactions of nitriles)
RN 78-94-4 HCAPLUS
CN 3-Buten-2-one (8CI, 9CI) (CA INDEX NAME)



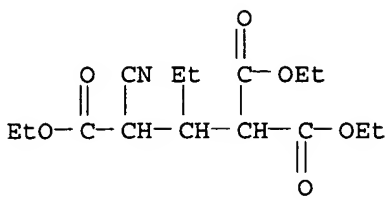
RN 121730-78-7 HCAPLUS
CN 1,1,3-Propanetricarboxylic acid, 3-cyano-2-methyl-, triethyl ester (9CI) (CA INDEX NAME)



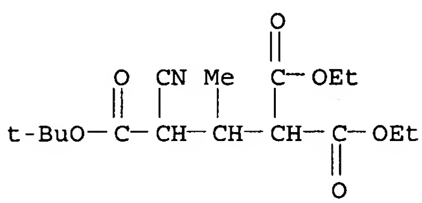
RN 173594-02-0 HCAPLUS
CN 1,1,3-Propanetricarboxylic acid, 3-cyano-2-methyl-, trimethyl ester (9CI) (CA INDEX NAME)



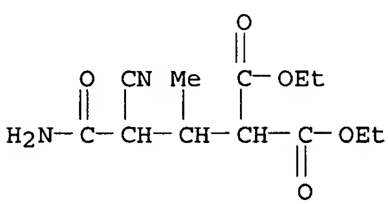
RN 173594-03-1 HCAPLUS
CN 1,1,3-Propanetricarboxylic acid, 3-cyano-2-ethyl-, triethyl ester (9CI) (CA INDEX NAME)



RN 173594-04-2 HCAPLUS
CN 1,1,3-Propanetricarboxylic acid, 3-cyano-2-methyl-, 3-(1,1-dimethylethyl) 1,1-diethyl ester (9CI) (CA INDEX NAME)

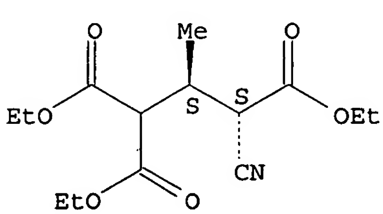


RN 173594-05-3 HCAPLUS
CN Propanedioic acid, (3-amino-2-cyano-1-methyl-3-oxopropyl)-, diethyl ester (9CI) (CA INDEX NAME)



IT **173593-73-2P 173593-75-4P 173593-87-8P**
173593-97-0P 173594-00-8P 173594-01-9P
173828-21-2P 173828-22-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(ruthenium-catalyzed aldol and Michael reactions of nitriles)
RN 173593-73-2 HCAPLUS
CN 1,1,3-Propanetricarboxylic acid, 3-cyano-2-methyl-, triethyl ester, (R*,R*)- (9CI) (CA INDEX NAME)

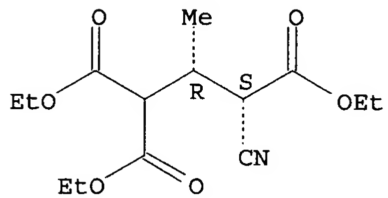
Relative stereochemistry.



RN 173593-75-4 HCAPLUS
CN 1,1,3-Propanetricarboxylic acid, 3-cyano-2-methyl-, triethyl

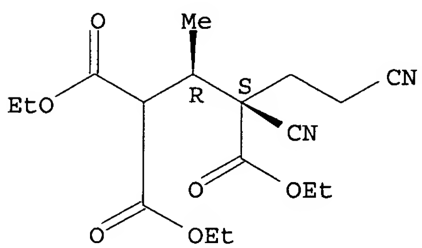
ester, (R*,S*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

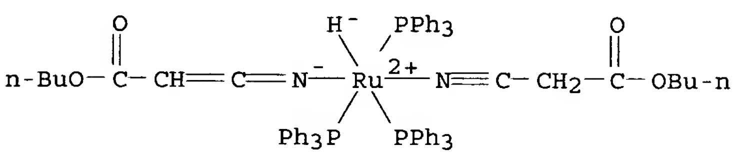


RN 173593-87-8 HCAPLUS
CN 1,1,3-Pentanetricarboxylic acid, 3,5-dicyano-2-methyl-, triethyl ester, (R*,S*)- (9CI) (CA INDEX NAME)

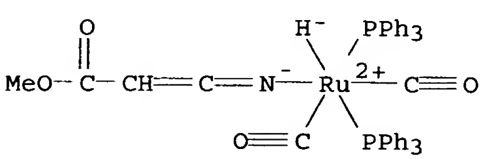
Relative stereochemistry.



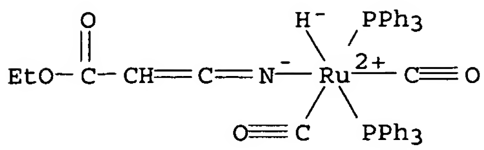
RN 173593-97-0 HCAPLUS
CN Ruthenium, (butyl cyanoacetate-N)(butyl 3-imino-2-propenoato-N)hydrotris(triphenylphosphine)-, (OC-6-31)- (9CI) (CA INDEX NAME)



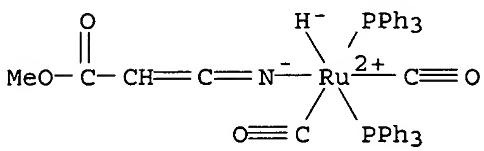
RN 173594-00-8 HCAPLUS
CN Ruthenium, dicarbonylhydro(methyl 3-imino-2-propenoato-N)bis(triphenylphosphine)-, (OC-6-13)- (9CI) (CA INDEX NAME)



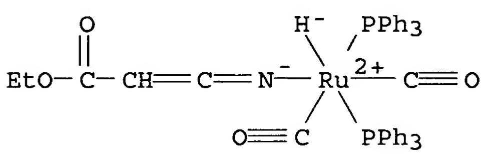
RN 173594-01-9 HCAPLUS
CN Ruthenium, dicarbonyl(ethyl 3-imino-2-propenoato-N)hydrobis(triphenylphosphine)-, (OC-6-13)- (9CI) (CA INDEX NAME)



RN 173828-21-2 HCAPLUS
CN Ruthenium, dicarbonylhydro(methyl 3-imino-2-propenoato-N)bis(triphenylphosphine)-, (OC-6-14)- (9CI) (CA INDEX NAME)



RN 173828-22-3 HCAPLUS
CN Ruthenium, dicarbonyl(ethyl 3-imino-2-propenoato-N)hydrobis(triphenylphosphine)-, (OC-6-14)- (9CI) (CA INDEX NAME)



CC 21-2 (General Organic Chemistry)
Section cross-reference(s): 22
IT Aldol condensation
Aldol condensation catalysts
Michael reaction
Michael reaction catalysts
Quantitative structure-activity relationship
(ruthenium-catalyzed aldol and Michael reactions of nitriles)
IT 121787-49-3P **173593-92-5P** 173593-93-6P
RL: BYP (Byproduct); PREP (Preparation)
(ruthenium-catalyzed aldol and Michael reactions of nitriles)
IT **138614-12-7P 138614-14-9P**
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(ruthenium-catalyzed aldol and Michael reactions of nitriles)
IT 74-88-4, Methyl iodide, reactions **78-94-4**, Methyl vinyl ketone, reactions 79-24-3, Nitroethane 96-33-3 100-50-5, 3-Cyclohexene-1-carboxaldehyde 100-52-7, Benzaldehyde, reactions 105-45-3, Methyl acetoacetate 105-56-6, Ethyl cyanoacetate 107-02-8, Acrolein, reactions 107-13-1, 2-Propenenitrile, reactions 108-59-8, Dimethyl malonate 108-94-1, Cyclohexanone, reactions 109-77-3, Dicyanomethane 123-08-0, 4-Hydroxybenzaldehyde 123-11-5, 4-Methoxybenzaldehyde, reactions 123-54-6, 2,4-Pentanedione, reactions 123-72-8, Butyraldehyde 140-29-4, Benzyl cyanide 140-88-5 495-41-0 538-51-2, N-Benzylideneaniline 623-47-2, Ethyl propiolate 627-26-9 630-08-0, Carbon monoxide, reactions 768-03-6, Phenyl vinyl ketone 1190-76-7 1423-60-5, Ethynyl methyl ketone 1462-12-0, Diethyl ethylidenemalonate 1572-99-2, Ethyl 2-cyanopropionate

1823-91-2, 2-Phenylpropionitrile 3696-36-4 5459-58-5, Butyl cyanoacetate 5832-70-2 17085-88-0, Diethyl propylidenemalonate 59853-02-0 **121730-78-7** **173594-02-0** **173594-03-1** **173594-04-2** **173594-05-3**
RL: RCT (Reactant); RACT (Reactant or reagent)
(ruthenium-catalyzed aldol and Michael reactions of nitriles)

IT 921-75-5P 1112-27-2P 2017-87-0P 2169-69-9P 4335-90-4P 4354-73-8P, Cyclohexylidenemalononitrile 6802-76-2P 14533-86-9P 14618-77-0P, Methyl 2-cyanopropanoate 15709-57-6P 30378-23-5P, Ethyl 2,4-dicyano-2-methylbutanoate 42205-38-9P 51067-99-3P 57812-20-1P 58774-06-4P 102746-75-8P, 2-Methyl-2-phenylpentanedinitrile 118745-25-8P, Ethyl (E)-2-cyano-2-hexenoate 118745-26-9P 118745-27-0P 121754-82-3P 155696-60-9P **173593-73-2P** 173593-74-3P **173593-75-4P** 173593-76-5P 173593-77-6P 173593-78-7P 173593-79-8P 173593-80-1P 173593-81-2P 173593-82-3P 173593-83-4P 173593-84-5P 173593-85-6P **173593-87-8P** 173593-88-9P 173593-89-0P 173593-91-4P 173593-94-7P 173593-95-8P 173593-96-9P **173593-97-0P** 173593-98-1P 173593-99-2P **173594-00-8P** **173594-01-9P** 173594-06-4P 173594-07-5P 173828-19-8P 173828-20-1P **173828-21-2P** **173828-22-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(ruthenium-catalyzed aldol and Michael reactions of nitriles)

L93 ANSWER 30 OF 34 HCAPLUS COPYRIGHT 2006 ACS on STN

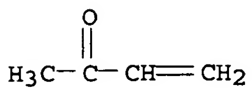
ACCESSION NUMBER: 1995:938755 HCAPLUS
DOCUMENT NUMBER: 124:55338
TITLE: Catalytic activity of polymerizable metal β-ketoesterato complexes towards Michael addition reactions
AUTHOR(S): Mastrorilli, P.; Nobile, C. F.; Suranna, G. P.
CORPORATE SOURCE: Centro di studi CNR sulle Metodologie Innovative in Sintesi Organiche M.I.S.O., Istituto di Chimica del Politecnico di Bari, trav. 200 Re David 4, Bari, I-70126, Italy
SOURCE: Journal of Molecular Catalysis A: Chemical (**1995**), 103(1), 23-9
CODEN: JMCCF2; ISSN: 1381-1169
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 124:55338

AB The addition of β-dioxo compds. R1C(O)CH2C(O)R2 (R1 = R2 = Me or OEt, R1 = Me, R2 = OMe) to Me vinyl ketone was catalyzed by Ni(II) and Co(II) complexes with the polymerizable β-ketoesterato 2-(acetoacetoxy)ethyl methacrylate (AAEMA-) under homogeneous and heterogeneous phases to give R1C(O)CH[C(O)R2]CH2CH2C(O)Me. The homogeneous reactions were carried out using the soluble Ni(AAEMA)2 and Co(AAEMA)2 complexes whereas the heterogeneous catalytic tests were carried out using the copolymers obtained by reaction of M(AAEMA)2 (M = Ni or Co) with suitable acrylamides. The Co(II) catalysts were more active than the Ni(II) catalysts in both the homogeneous and heterogeneous phases.

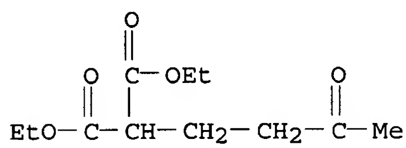
ED Entered STN: 23 Nov 1995

IT **78-94-4**, Methyl vinyl ketone, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(Michael addition of β-dioxo compds. with Me vinyl ketone catalyzed by nickel and cobalt (acetoacetoxy)ethyl methacrylate complexes and their acrylamide copolymers)

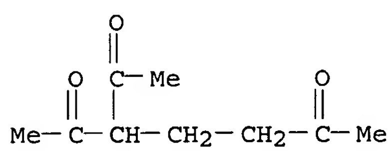
RN 78-94-4 HCAPLUS
CN 3-Buten-2-one (8CI, 9CI) (CA INDEX NAME)



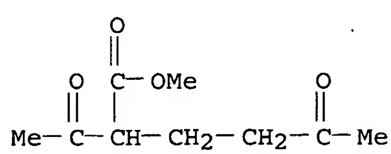
IT **4761-26-6P 29214-57-1P**, 3-Acetylheptane-2,6-
dione **35490-04-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(Michael addition of β-dioxo compds. with Me vinyl ketone catalyzed by nickel and cobalt (acetoacetoxy)ethyl methacrylate complexes and their acrylamide copolymers)
RN 4761-26-6 HCAPLUS
CN Propanedioic acid, (3-oxobutyl)-, diethyl ester (9CI) (CA INDEX NAME)



RN 29214-57-1 HCAPLUS
CN 2,6-Heptanedione, 3-acetyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



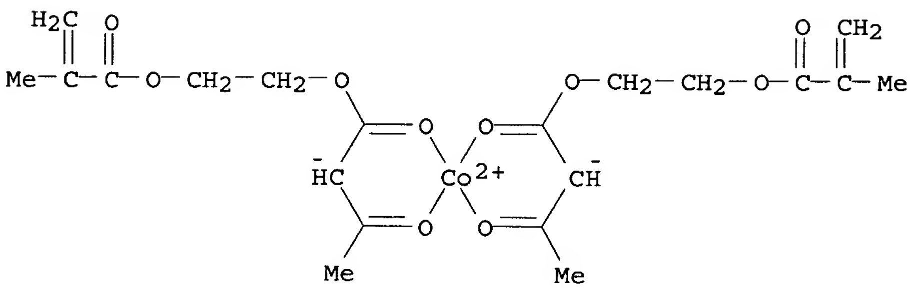
RN 35490-04-1 HCAPLUS
CN Hexanoic acid, 2-acetyl-5-oxo-, methyl ester (9CI) (CA INDEX NAME)



IT **172172-22-4P 172172-23-5P**
RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(preparation as catalyst for Michael addition of β-dioxo compds. with Me vinyl ketone)
RN 172172-22-4 HCAPLUS
CN Cobalt, bis[[(2-methyl-1-oxo-2-propenyl)oxy]ethyl 3-(oxo-κO)butanoato-κO']-, polymer with N,N-dimethyl-2-propenamide and N,N'-methylenebis[2-propenamide] (9CI) (CA INDEX NAME)

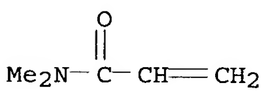
CM 1

CRN 156127-94-5
CMF C20 H26 Co O10
CCI CCS



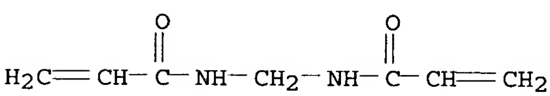
CM 2

CRN 2680-03-7
CMF C5 H9 N O



CM 3

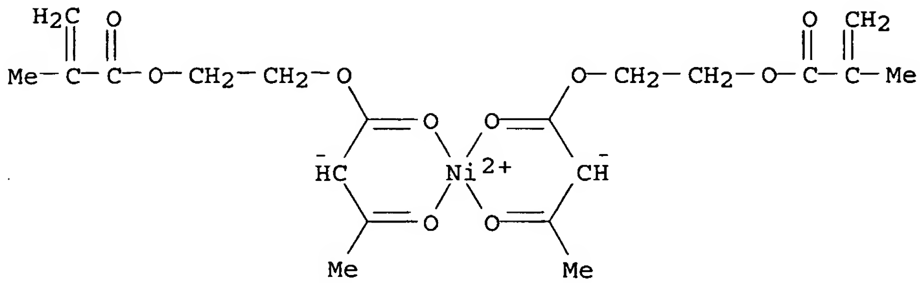
CRN 110-26-9
CMF C7 H10 N2 O2



RN 172172-23-5 HCAPLUS
CN Nickel, bis[[(2-methyl-1-oxo-2-propenyl)oxy]ethyl 3-oxobutanoato-O1,O3]-, polymer with N,N-dimethyl-2-propenamide and N,N'-methylenebis[2-propenamide] (9CI) (CA INDEX NAME)

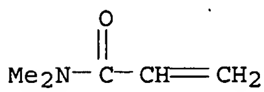
CM 1

CRN 156127-92-3
CMF C20 H26 Ni O10
CCI CCS



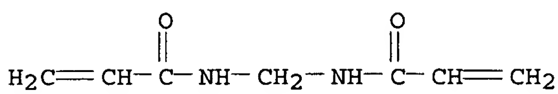
CM 2

CRN 2680-03-7
CMF C5 H9 N O



CM 3

CRN 110-26-9
CMF C7 H10 N2 O2

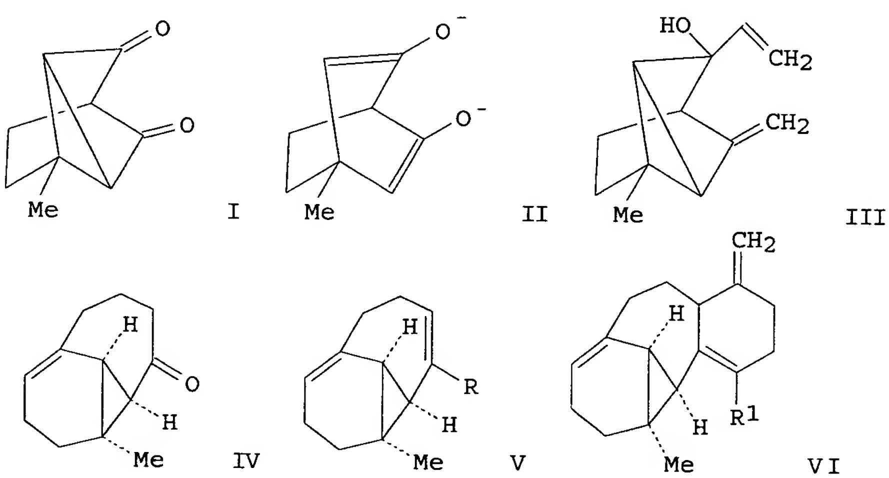


CC 23-17 (Aliphatic Compounds)
Section cross-reference(s): 35, 67
IT **Michael reaction catalysts**
(nickel and cobalt (acetoacetoxy)ethyl methacrylate complexes and their acrylamide copolymers for β-dioxo compds. with Me vinyl ketone)
IT **78-94-4**, Methyl vinyl ketone, reactions 105-45-3, Methyl acetoacetate 105-53-3, Diethyl malonate 123-54-6, 2,4-Pentanedione, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(Michael addition of β-dioxo compds. with Me vinyl ketone catalyzed by nickel and cobalt (acetoacetoxy)ethyl methacrylate complexes and their acrylamide copolymers)
IT **4761-26-6P 29214-57-1P**, 3-Acetylheptane-2,6-dione **35490-04-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(Michael addition of β-dioxo compds. with Me vinyl ketone catalyzed by nickel and cobalt (acetoacetoxy)ethyl methacrylate complexes and their acrylamide copolymers)
IT **172172-22-4P 172172-23-5P**
RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(preparation as catalyst for Michael addition of β-dioxo compds.

with Me vinyl ketone)

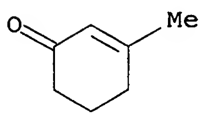
L93 ANSWER 31 OF 34 HCAPLUS

ACCESSION NUMBER: 1993:581045 HCAPLUS
DOCUMENT NUMBER: 119:181045
TITLE: Studies directed toward the total synthesis of cerorubenic acid-III. 1. Expedient construction of the tetracyclic core by oxyanionic sigmatropy
AUTHOR(S): Paquette, Leo A.; Poupart, Marc Andre
CORPORATE SOURCE: Evans Chem. Lab., Ohio State Univ., Columbus, OH, 43210, USA
SOURCE: Journal of Organic Chemistry (1993), 58(16), 4245-53
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 119:181045
GI

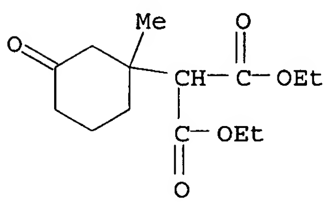


AB A synthesis of the ABCD ring framework of cerorubenic acid-III is described. Diketone I was first prepared by intramol. oxidative coupling of the dienolate II and then suitably desymmetrized to deliver III. Anionic oxy-Cope rearrangement of this intermediate resulted in construction of IV, a ketone not only having all three contiguous stereogenic centers properly established but also equipped with adequate functionality for the further elaboration of ring D. In the present effort, this thrust took the form of homologation to V (R = Ac), conversion to the activated diene V [R = C(OSiMe2CMe3):CH2], and Diels-Alder cycloaddn. to Me acrylate at high pressure. Once it became obvious that first-formed ketone greatly preferred adoption of trans stereochem. at the ring juncture, attempts to skirt this issue were made by preparing both VI (R1 = CN) and VI (R1 = Ac). However, these advanced intermediates proved unresponsive to conjugate reduction, and attention was therefore redirected to alternative possible means for elaboration of the eastern sector.

ED Entered STN: 30 Oct 1993
IT **1193-18-6**
RL: RCT (Reactant); **RACT (Reactant or reagent)**
(conjugate vinylation or Michael addition to, by malonate)
RN 1193-18-6 HCAPLUS
CN 2-Cyclohexen-1-one, 3-methyl- (7CI, 8CI, 9CI) (CA INDEX NAME)

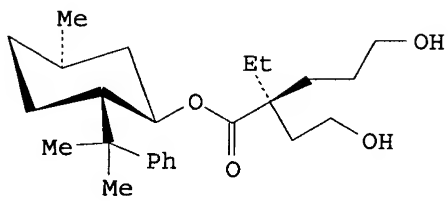
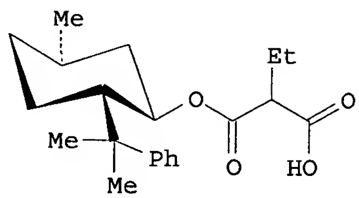


IT **88710-73-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP
(Preparation); RACT (Reactant or reagent)
(preparation, saponification, and decarboxylation of)
RN 88710-73-0 HCAPLUS
CN Propanedioic acid, (1-methyl-3-oxocyclohexyl)-, diethyl ester
(9CI) (CA INDEX NAME)



CC 30-25 (Terpenes and Terpenoids)
IT **Asymmetric synthesis and induction**
(of cerorubenic acid-III tetracyclic core)
IT **1193-18-6**
RL: RCT (Reactant); **RACT (Reactant or reagent)**
(conjugate vinylation or Michael addition to, by malonate)
IT **88710-73-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP
(Preparation); RACT (Reactant or reagent)
(preparation, saponification, and decarboxylation of)

L93 ANSWER 32 OF 34 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1992:571787 HCAPLUS
DOCUMENT NUMBER: 117:171787
TITLE: Enantioselective construction of a quaternary stereogenic center via tandem acid anhydride formation-intramolecular Michael reaction
AUTHOR(S): Ihara, Masataka; Taniguchi, Nobuaki; Suzuki, Shuichi; Fukumoto, Keiichiro
CORPORATE SOURCE: Pharm. Inst., Tohoku Univ., Sendai, 980, Japan
SOURCE: Journal of the Chemical Society, Chemical Communications (**1992**), (14), 976-7
CODEN: JCCCAT; ISSN: 0022-4936
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 117:171787
GI


I

II

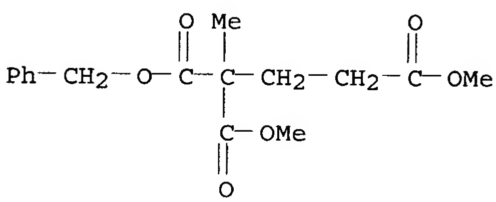
AB A novel method for the enantioselective construction of a quaternary stereogenic center by tandem acid anhydride formation-intramol. Michael reaction has been developed; a synthetic intermediate I for Hunteria and Aspidosperma indole alkaloids has been prepared by the application of this procedure using acid II and acryloyl chloride.

ED Entered STN: 01 Nov 1992

IT **143723-43-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 143723-43-7 HCAPLUS

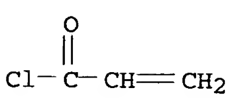
CN 1,3,3-Butanetricarboxylic acid, 1,3-dimethyl 3-(phenylmethyl) ester (9CI) (CA INDEX NAME)



IT **814-68-6**, Acryloyl chloride
RL: RCT (Reactant); **RACT (Reactant or reagent)**
(reaction of, with chiral half ester and subsequent intramol. Michael reaction)

RN 814-68-6 HCAPLUS

CN 2-Propenoyl chloride (9CI) (CA INDEX NAME)



CC 31-5 (Alkaloids)
Section cross-reference(s): 22

IT **Asymmetric synthesis and induction**
(in tandem acid anhydride formation-intramol. Michael reaction)

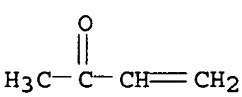
IT **Michael reaction**
(intramol., tandem acid anhydride formation and, in synthesis of indole alkaloid intermediate)

IT 123463-89-8P 132143-23-8P **143723-43-7P** 143723-44-8P 143723-45-9P 143723-48-2P 143723-50-6P 143723-53-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

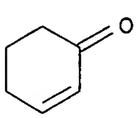
IT **814-68-6**, Acryloyl chloride

RL: RCT (Reactant); **RACT (Reactant or reagent)**
(reaction of, with chiral half ester and subsequent intramol. Michael reaction)

L93 ANSWER 33 OF 34 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1991:142264 HCAPLUS
DOCUMENT NUMBER: 114:142264
TITLE: Michael addition promoted by bis-bidentate nickel(II) Schiff base complexes derived from aromatic 2-hydroxy aldehydes
AUTHOR(S): Botteghi, C.; Schionato, A.; Rosini, C.; Salvadori, P.
CORPORATE SOURCE: Dip. Chim., Univ. Venezia, Venice, 30123, Italy
SOURCE: Journal of Molecular Catalysis (**1990**), 63(2), 155-65
CODEN: JMCADS; ISSN: 0304-5102
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 114:142264
AB Bis-bidentate Ni(II) Schiff-base complexes derived from 2-HOC6H4CHO or hydroxynaphthaldehydes catalyze the Michael addition of β-oxo esters to MeCOCH:CH2. Complexes with prevailing square-planar structure in solution are more active than their tetrahedral isomers. Low optical inductions (≤6%) are observed only if the Michael addns. are carried out in the presence of square-planar complexes with optically active Schiff-base ligands.
ED Entered STN: 19 Apr 1991
IT **78-94-4**, Methyl vinyl ketone, reactions **930-68-7**, 2-Cyclohexen-1-one
RL: RCT (Reactant); RACT (Reactant or reagent)
(Michael addition reaction of, with dicarbonyl compds., catalysts for)
RN 78-94-4 HCAPLUS
CN 3-Buten-2-one (8CI, 9CI) (CA INDEX NAME)

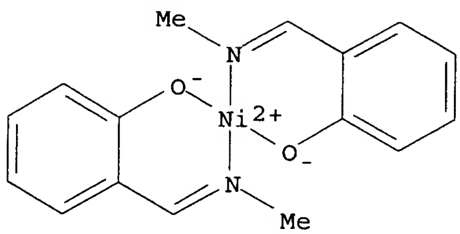


RN 930-68-7 HCAPLUS
CN 2-Cyclohexen-1-one (6CI, 8CI, 9CI) (CA INDEX NAME)

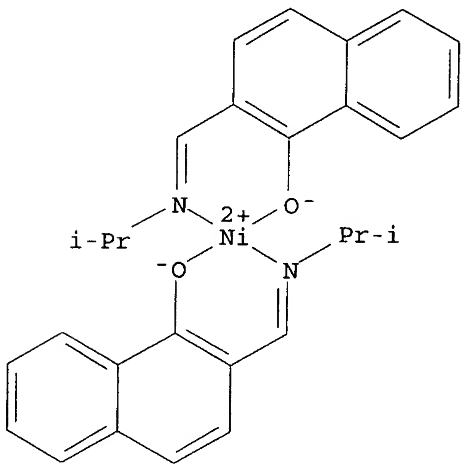


IT **14322-02-2 15379-94-9 15390-05-3**
56647-29-1 56647-30-4
RL: CAT (Catalyst use); USES (Uses)
(catalyst, for Michael addition reaction of dicarbonyl compds. with unsatd. ketones)
RN 14322-02-2 HCAPLUS
CN Nickel, bis[2-[(methylimino-κN)methyl]phenolato-κO]-

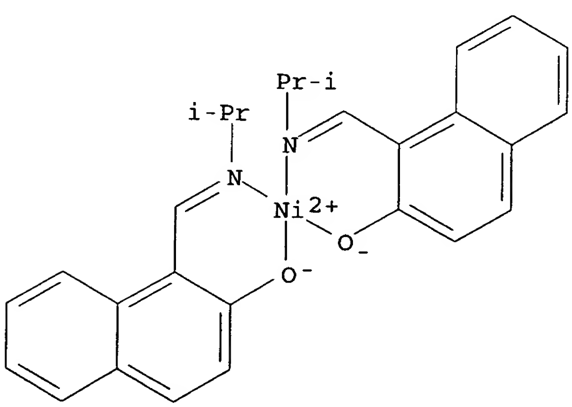
(9CI) (CA INDEX NAME)



RN 15379-94-9 HCAPLUS
CN Nickel, bis[2-[[(1-methylethyl)imino]methyl]-1-naphthalenolato-
N,O]- (9CI) (CA INDEX NAME)

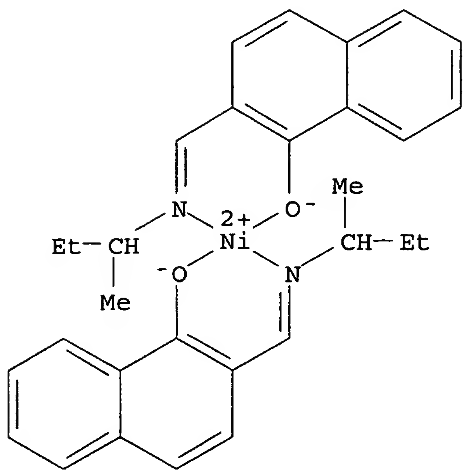


RN 15390-05-3 HCAPLUS
CN Nickel, bis[1-[[(1-methylethyl)imino]methyl]-2-naphthalenolato-
N,O]- (9CI) (CA INDEX NAME)

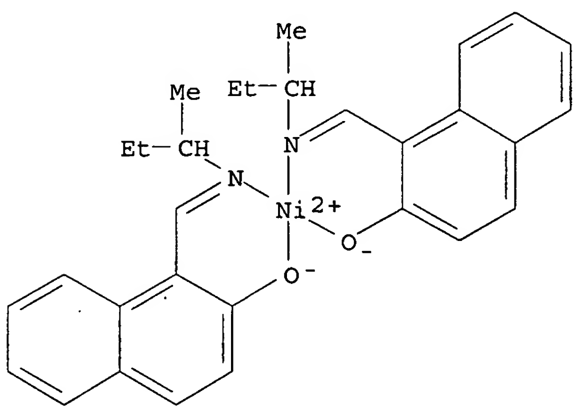


RN 56647-29-1 HCAPLUS
CN Nickel, bis[2-[[(1-methylpropyl)imino]methyl]-1-naphthalenolato-

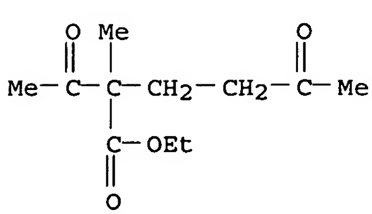
N,O]-, [T-4-(S),(S)]- (9CI) (CA INDEX NAME)



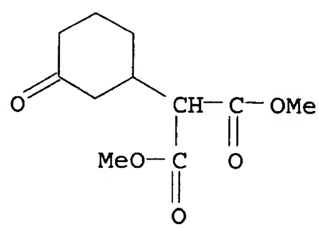
RN 56647-30-4 HCAPLUS
CN Nickel, bis[1-[[(1-methylpropyl)imino]methyl]-2-naphthalenolato-
N,O]-, [SP-4-1-(S),(S)]- (9CI) (CA INDEX NAME)



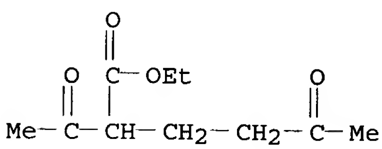
IT **28793-08-0P 33646-18-3P 35490-05-2P**
66152-63-4P 78044-62-9P 94410-52-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 28793-08-0 HCAPLUS
CN Hexanoic acid, 2-acetyl-2-methyl-5-oxo-, ethyl ester (6CI, 8CI,
9CI) (CA INDEX NAME)



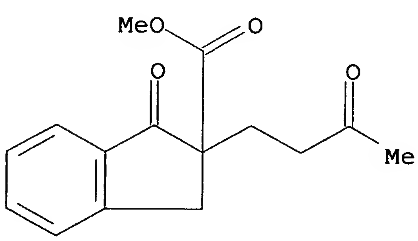
RN 33646-18-3 HCAPLUS
CN Propanedioic acid, (3-oxocyclohexyl)-, dimethyl ester (9CI) (CA INDEX NAME)



RN 35490-05-2 HCAPLUS
CN Hexanoic acid, 2-acetyl-5-oxo-, ethyl ester (6CI, 7CI, 9CI) (CA INDEX NAME)

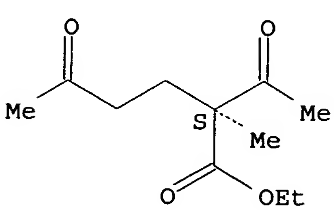


RN 66152-63-4 HCAPLUS
CN 1H-Indene-2-carboxylic acid, 2,3-dihydro-1-oxo-2-(3-oxobutyl)-, methyl ester (9CI) (CA INDEX NAME)



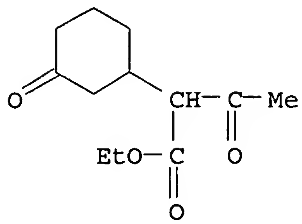
RN 78044-62-9 HCAPLUS
CN Hexanoic acid, 2-acetyl-2-methyl-5-oxo-, ethyl ester, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



RN 94410-52-3 HCAPLUS
CN Cyclohexaneacetic acid, α-acetyl-3-oxo-, ethyl ester (9CI)

(CA INDEX NAME)



CC 21-2 (General Organic Chemistry)
Section cross-reference(s): 25

IT **Michael reaction catalysts**
(nickel complexes of Schiff bases derived from aromatic hydroxy aldehydes, for dicarbonyl compds. with unsatd. ketones)

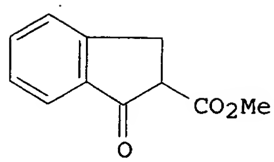
IT **Michael reaction**
(of dicarbonyl compds. with unsatd. ketones, catalytic)

IT **78-94-4**, Methyl vinyl ketone, reactions **930-68-7**, 2-Cyclohexen-1-one
RL: RCT (Reactant); RACT (Reactant or reagent)
(Michael addition reaction of, with dicarbonyl compds., catalysts for)

IT **14322-02-2 15379-94-9 15390-05-3**
56647-29-1 56647-30-4
RL: CAT (Catalyst use); USES (Uses)
(catalyst, for Michael addition reaction of dicarbonyl compds. with unsatd. ketones)

IT **28793-08-0P 33646-18-3P 35490-05-2P**
66152-63-4P 78044-62-9P 94410-52-3P
132931-89-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

L93 ANSWER 34 OF 34 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1984:209326 HCAPLUS
DOCUMENT NUMBER: 100:209326
TITLE: Asymmetric catalyses. Part 18. Enantioselective Michael additions using optically active cobalt(II)/diamine catalysts
AUTHOR(S): Brunner, Henri; Hammer, Benedikt
CORPORATE SOURCE: Inst. Anorg. Chem., Univ. Regensburg, Regensburg, D-8400, Fed. Rep. Ger.
SOURCE: Angewandte Chemie (**1984**), 96(4), 305-6
CODEN: ANCEAD; ISSN: 0044-8249
DOCUMENT TYPE: Journal
LANGUAGE: German
GI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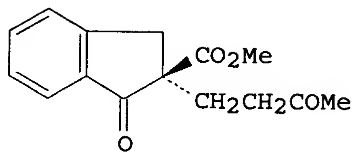
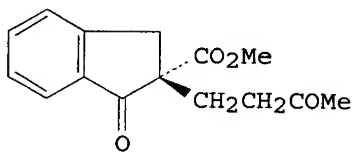

II


III

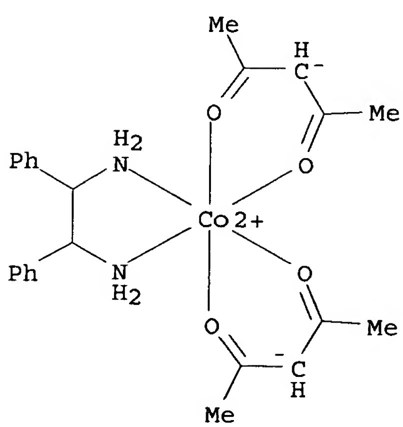
AB Co(acac)2(nn) [acac = MeCOCH2COMe, nn = (+)- or (-)-H2NCHPhCHPhNH2] catalyzed the enantioselective Michael addition of H2C:CHCOMe to indancarboxylate I to give the addition product II or III in enantiomeric excess (ee). H2C:CHCOMe added to I in 40 h at 20° with Co(acac)2[(+)-nn] to give 79% yield of II with 21.3% ee. This ee yield increased with decreasing temperature to 66% ee at -50° in 64 h. (-)-(Nn) gave 5.8% ee of II at 20° but Co(acac)2[(-)-nn] gave 37.2 and 58.3% ee of III at -20 and -40°, resp. H2C:CHCOMe and MeCOCHMeCO2Et under Co(acac)2[(+)-nn] catalysis gave 4.5% ee of Michael adduct at room temperature

ED Entered STN: 23 Jun 1984

IT **89485-98-3**
RL: CAT (Catalyst use); USES (Uses)
(catalyst, for enantioselective Michael addition of indancarboxylate with 1,3-dicarbonyl compds.)

RN 89485-98-3 HCAPLUS

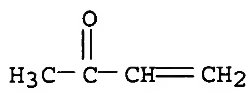
CN Cobalt, (1,2-diphenyl-1,2-ethanediamine-N,N')bis(2,4-pentanedionato-O,O')-, [OC-6-21-[S-(R*,R*)]]- (9CI) (CA INDEX NAME)



IT **78-94-4**, reactions
RL: RCT (Reactant); **RACT (Reactant or reagent)**
(enantioselective Michael addition reaction of, with indancarboxylate in presence of cobalt(II)-optically active diamines)

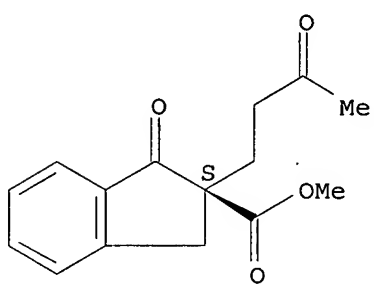
RN 78-94-4 HCAPLUS

CN 3-Buten-2-one (8CI, 9CI) (CA INDEX NAME)



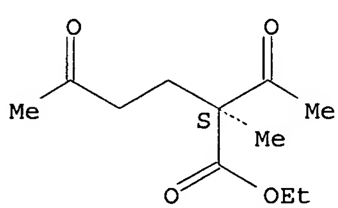
IT **58623-84-0P 78044-62-9P 79298-08-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 58623-84-0 HCAPLUS
CN 1H-Indene-2-carboxylic acid, 2,3-dihydro-1-oxo-2-(3-oxobutyl)-, methyl ester, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



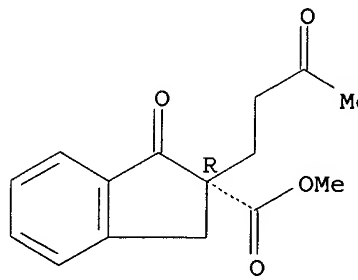
RN 78044-62-9 HCAPLUS
CN Hexanoic acid, 2-acetyl-2-methyl-5-oxo-, ethyl ester, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



RN 79298-08-1 HCAPLUS
CN 1H-Indene-2-carboxylic acid, 2,3-dihydro-1-oxo-2-(3-oxobutyl)-, methyl ester, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



CC 25-23 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
Section cross-reference(s): 22

IT **Asymmetric synthesis and induction**
(Michael adducts, of indancarboxylates with 1,3-dicarbonyl compds. in presence of cobalt(II)-optically active diamine catalysts)

IT **Michael reaction catalysts**
(cobalt(II)-optically active diamines, for indancarboxylates with 1,3-dicarbonyl compds.)

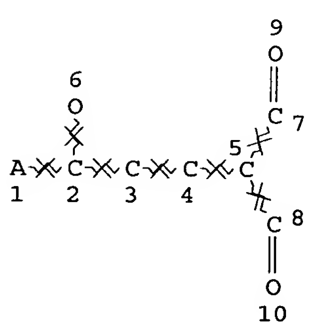
IT **Michael reaction**
(enantioselective, of indancarboxylates with 1,3-dicarbonyl compds.)

IT **89485-98-3**
RL: CAT (Catalyst use); USES (Uses)
(catalyst, for enantioselective Michael addition of indancarboxylate with 1,3-dicarbonyl compds.)

IT **78-94-4**, reactions 609-14-3
RL: RCT (Reactant); **RACT (Reactant or reagent)**
(enantioselective Michael addition reaction of, with indancarboxylate in presence of cobalt(II)-optically active diamines)

IT **58623-84-0P 78044-62-9P 79298-08-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

=> => d que l111
L21 SCR 1918 OR 2043 OR 1840 OR 1949 OR 2010
L25 STR

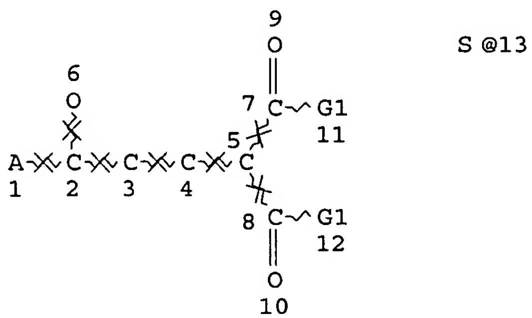


NODE ATTRIBUTES:
CONNECT IS X2 RC AT 6
CONNECT IS E1 RC AT 9
CONNECT IS E1 RC AT 10

DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 10

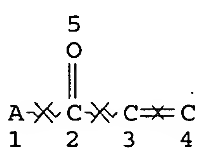
STEREO ATTRIBUTES: NONE
L27 12118 SEA FILE=REGISTRY SSS FUL L25 NOT L21
L30 STR



VAR G1=O/N/P/13
NODE ATTRIBUTES:
CONNECT IS X2 RC AT 6
CONNECT IS E1 RC AT 9
CONNECT IS E1 RC AT 10
CONNECT IS X2 RC AT 13
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 13

STEREO ATTRIBUTES: NONE
L32 2503 SEA FILE=REGISTRY SUB=L27 SSS FUL L30
L37 STR



NODE ATTRIBUTES:
CONNECT IS E1 RC AT 5
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 5

STEREO ATTRIBUTES: NONE
L40 SCR 1918 OR 2043 OR 1839 OR 1944 OR 2005
L42 6815 SEA FILE=REGISTRY SSS FUL L37 NOT L40
L106 816 SEA FILE=CAOLD ABB=ON PLU=ON L27
L107 175 SEA FILE=CAOLD ABB=ON PLU=ON L32

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L108        1649 SEA FILE=CAOLD ABB=ON  PLU=ON  L42
L109          21 SEA FILE=CAOLD ABB=ON  PLU=ON  L106 AND L108
L110           6 SEA FILE=CAOLD ABB=ON  PLU=ON  L108 AND L107
L111          21 SEA FILE=CAOLD ABB=ON  PLU=ON  L109 OR L110
```

```
=> d l111 1-21 iall hitstr hitind
```

```
L111 ANSWER 1 OF 21  CAOLD  COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER:   CA63:8636c  CAOLD
TITLE:              tryptophan metabolism
AUTHOR NAME:        Scott, Thomas Arthur
INDEX TERM:           57-57-8      67-47-0      78-94-4
                    108-30-5     128-53-0     151-56-4     498-23-7
                    520-45-6     551-16-6     616-02-4     768-03-6
                    872-36-6    2170-03-8
IT    78-94-4    520-45-6
RN    78-94-4  CAOLD
CN    3-Buten-2-one (8CI, 9CI)  (CA INDEX NAME)
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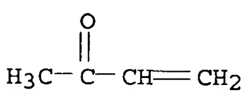

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RN    520-45-6  CAOLD
CN    2H-Pyran-2,4(3H)-dione, 3-acetyl-6-methyl- (8CI, 9CI)  (CA INDEX
      NAME)
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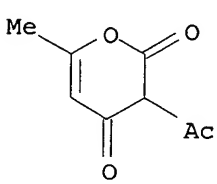

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IT     57-57-8     67-47-0     78-94-4     108-30-5
      128-53-0    151-56-4    498-23-7     520-45-6    551-16-6
      616-02-4    768-03-6    872-36-6    2170-03-8
```

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L111 ANSWER 2 OF 21  CAOLD  COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER:   CA62:16042e  CAOLD
TITLE:              expts. in the synthesis of structure related to ring
                    A of the triterpenes
AUTHOR NAME:        Baisted, Derek J.; Whitehurst, J. S.
INDEX TERM:         1216-53-1    1606-24-2    1606-25-3    1606-26-4
                    1606-27-5    1606-45-7    1606-47-9
                    1609-24-1    1609-25-2    1839-40-3    1839-41-4
                    1839-42-5    1944-81-6    1944-82-7
                    2020-06-6    2020-07-7    2020-08-8    2020-09-9
                    2020-10-2    2020-11-3    2020-12-4
                    2020-13-5    2020-14-6    2020-15-7
                    2020-16-8    2020-17-9    2020-18-0    2020-21-5
                    2092-35-5    2092-36-6    2278-89-9
                    2390-14-9    2420-83-9    3333-39-9    3425-62-5
                    3425-63-6    3425-64-7    3425-65-8    3425-66-9
                    3425-67-0    3425-68-1    3425-69-2    3425-70-5
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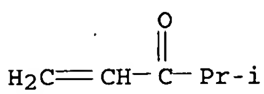
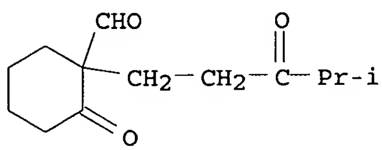
3425-71-6   3505-66-6   3758-40-5   4006-21-7
93997-67-2   96168-60-4   **98763-68-9**
99871-63-3   100658-59-1

IT   **1606-47-9**   **1944-81-6**   **2020-12-4**
2020-14-6   **2092-35-5**   **98763-68-9**

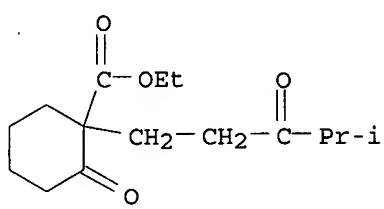
RN   1606-47-9   CAOLD
CN   1-Penten-3-one, 4-methyl- (8CI, 9CI)   (CA INDEX NAME)



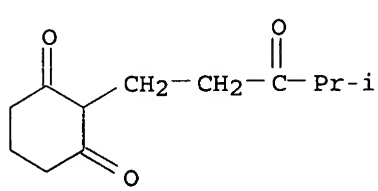
RN   1944-81-6   CAOLD
CN   Cyclohexanecarboxaldehyde, 1-(4-methyl-3-oxopentyl)-2-oxo- (7CI, 8CI)   (CA INDEX NAME)



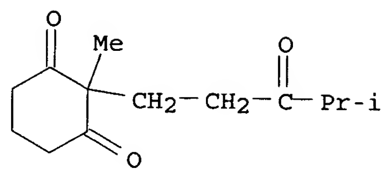
RN   2020-12-4   CAOLD
CN   Cyclohexanecarboxylic acid, 1-(4-methyl-3-oxopentyl)-2-oxo-, ethyl ester (7CI, 8CI)   (CA INDEX NAME)



RN   2020-14-6   CAOLD
CN   1,3-Cyclohexanedione, 2-(4-methyl-3-oxopentyl)- (7CI, 8CI)   (CA INDEX NAME)



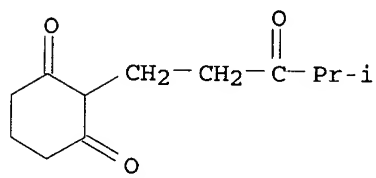
RN   2092-35-5   CAOLD
CN   1,3-Cyclohexanedione, 2-methyl-2-(4-methyl-3-oxopentyl)- (7CI, 8CI, 9CI)   (CA INDEX NAME)



RN 98763-68-9 CAOLD
CN 1,3-Cyclohexanedione, 2-(4-methyl-3-oxopentyl)-, (2,4-dinitrophenyl)hydrazone (7CI) (CA INDEX NAME)

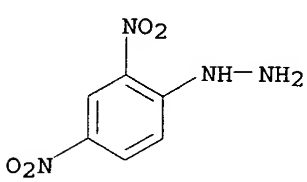
CM 1

CRN 2020-14-6
CMF C12 H18 O3



CM 2

CRN 119-26-6
CMF C6 H6 N4 O4



IT **1216-53-1** **1606-24-2** **1606-25-3**
1606-26-4 **1606-27-5** **1606-45-7**
1606-47-9 1609-24-1 1609-25-2 1839-40-3 1839-41-4
1839-42-5 1944-81-6 1944-82-7 2020-06-6 2020-07-7
2020-08-8 2020-09-9 2020-10-2 2020-11-3 2020-12-4
2020-13-5 2020-14-6 2020-15-7 2020-16-8 2020-17-9
2020-18-0 2020-21-5 2092-35-5 2092-36-6 2278-89-9
2390-14-9 2420-83-9 3333-39-9 3425-62-5 3425-63-6
3425-64-7 3425-65-8 3425-66-9 3425-67-0 3425-68-1
3425-69-2 3425-70-5 3425-71-6 3505-66-6 3758-40-5
4006-21-7 93997-67-2 96168-60-4 98763-68-9 99871-63-3
100658-59-1

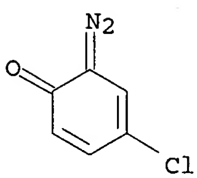
L111 ANSWER 3 OF 21 CAOLD
ACCESSION NUMBER: CA62:7903d CAOLD
TITLE: reactions with diazocarbonyl compds. - (XIV) o-quinone triaminophosphazines
AUTHOR NAME: Ried, Walter; Appel. H.

INDEX TERM:	1201-33-8	3028-26-0	**3028-27-1**	
	3028-29-3	**3028-30-6**	3028-31-7	
	3028-32-8	3028-33-9	3028-34-0	3028-35-1
	3028-36-2	3028-37-3	3028-38-4	3028-39-5
	3028-40-8	3028-41-9	3028-42-0	3028-43-1
	3028-44-2	**3028-45-3**	3028-46-4	
	3028-47-5	3028-48-6	3028-49-7	3028-50-0
	3028-51-1	3028-52-2	3028-53-3	3028-54-4
	3028-55-5	3028-56-6	3028-57-7	3028-58-8
	3028-59-9	3028-60-2	3028-63-5	3028-64-6
	3028-65-7	3028-66-8	3028-67-9	3028-68-0
	3028-69-1	3028-70-4	3028-71-5	3028-72-6
	3028-73-7	3061-79-8	3065-35-8	3065-36-9
	3089-74-5	3089-80-3	3089-81-4	3089-82-5
	3374-09-2	3374-10-5	3441-66-5	3441-76-7
	3441-77-8	3441-78-9	3441-79-0	3442-16-8
	3577-41-1	3577-42-2	3978-36-7	

IT **3028-27-1** **3028-30-6** **3028-45-3**

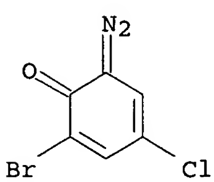
RN 3028-27-1 CAOLD

CN 2,4-Cyclohexadien-1-one, 4-chloro-6-diazo- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



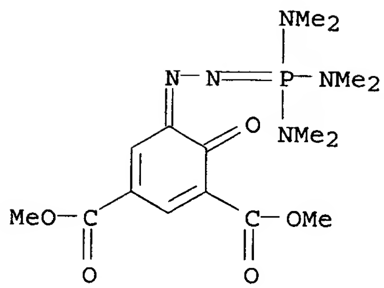
RN 3028-30-6 CAOLD

CN 2,4-Cyclohexadien-1-one, 2-bromo-4-chloro-6-diazo- (7CI, 8CI) (CA INDEX NAME)



RN 3028-45-3 CAOLD

CN Phosphorane, [(3,5-dicarboxy-6-oxo-2,4-cyclohexadien-1-ylidene)hydrazono]tris(dimethylamino)-, dimethyl ester (7CI, 8CI) (CA INDEX NAME)



IT **1201-33-8** **3028-26-0** **3028-27-1**
3028-29-3 3028-30-6 3028-31-7 3028-32-8 3028-33-9
3028-34-0 3028-35-1 3028-36-2 3028-37-3 3028-38-4
3028-39-5 3028-40-8 3028-41-9 3028-42-0 3028-43-1
3028-44-2 3028-45-3 3028-46-4 3028-47-5 3028-48-6
3028-49-7 3028-50-0 3028-51-1 3028-52-2 3028-53-3
3028-54-4 3028-55-5 3028-56-6 3028-57-7 3028-58-8
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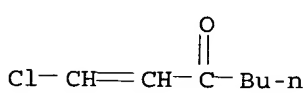
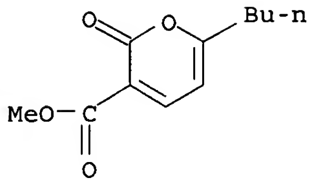
3065-36-9 3089-74-5 3089-80-3 3089-81-4 3089-82-5
3374-09-2 3374-10-5 3441-66-5 3441-76-7 3441-77-8
3441-78-9 3441-79-0 3442-16-8 3577-41-1 3577-42-2
3978-36-7

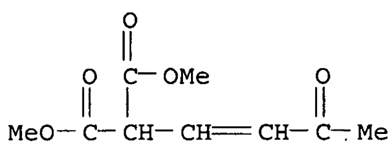
L111 ANSWER 4 OF 21 CAOLD
ACCESSION NUMBER: CA62:3997g CAOLD
TITLE: intramol. cyclization of alkylpropargylidenemalonic acids-catalytic and directing effect of Ag ion
AUTHOR NAME: Belil, C.; Pascual, J.; Serratosa, F.
INDEX TERM: 921-46-0 921-86-8 922-87-2 922-90-7
924-95-8 936-09-4 946-67-8 1069-35-8
1137-22-0 **1186-86-3** 1196-35-6
1213-20-3 **1920-22-5** 2052-89-3
IT **924-95-8** **1137-22-0** **1186-86-3**
1920-22-5
RN 924-95-8 CAOLD
CN 1-Hepten-3-one, 1-chloro- (7CI, 8CI, 9CI) (CA INDEX NAME)



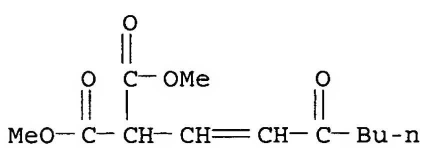
RN 1137-22-0 CAOLD
CN Malonic acid, (3-hydroxy-2-heptenylidene)-, δ-lactone, methyl ester (7CI, 8CI) (CA INDEX NAME)



RN 1186-86-3 CAOLD
CN Malonic acid, (3-oxo-1-butenyl)-, dimethyl ester (7CI, 8CI) (CA INDEX NAME)

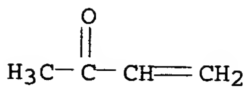


RN 1920-22-5 CAOLD
CN Malonic acid, (3-oxo-1-heptenyl)-, dimethyl ester (7CI, 8CI) (CA INDEX NAME)

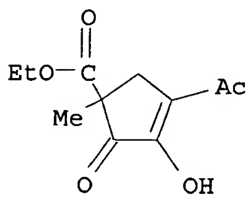


IT **921-46-0** **921-86-8** **922-87-2**
922-90-7 924-95-8 936-09-4 946-67-8 1069-35-8
1137-22-0 1186-86-3 1196-35-6 1213-20-3 1920-22-5
2052-89-3

L111 ANSWER 5 OF 21 CAOLD COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: CA62:2717b CAOLD
TITLE: course of the Michael aldol synthesis - (I) formation of cyclopentanediones, (II) of cyclohexenones
AUTHOR NAME: Goldsmith, David J.; Hartman, J. A.
INDEX TERM: **78-94-4** 183-97-1 759-65-9
765-70-8 769-45-9 769-46-0 771-74-4
778-06-3 **780-73-4** **783-70-0**
786-14-1 889-67-8 **26103-79-7**
91062-15-6 **92723-62-1** 94520-21-5
96080-97-6 **96380-22-2**
IT **78-94-4** **780-73-4** **783-70-0**
786-14-1 **26103-79-7** **92723-62-1**
96380-22-2
RN 78-94-4 CAOLD
CN 3-Buten-2-one (8CI, 9CI) (CA INDEX NAME)

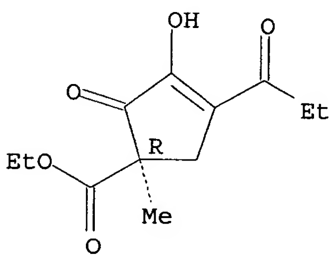


RN 780-73-4 CAOLD
CN 3-Cyclopentene-1-carboxylic acid, 4-acetyl-3-hydroxy-1-methyl-2-oxo-, ethyl ester (7CI, 8CI) (CA INDEX NAME)



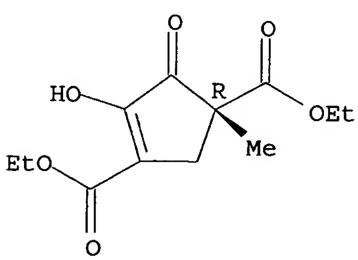
RN 783-70-0 CAOLD
CN 3-Cyclopentene-1-carboxylic acid, 3-hydroxy-1-methyl-2-oxo-4-propionyl-, ethyl ester, (R)- (8CI) (CA INDEX NAME)

Absolute stereochemistry.

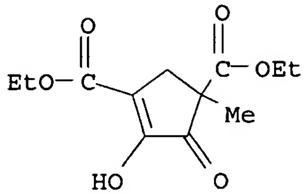


RN 786-14-1 CAOLD
CN 3-Cyclopentene-1,3-dicarboxylic acid, 4-hydroxy-1-methyl-5-oxo-, diethyl ester, (R)- (9CI) (CA INDEX NAME)

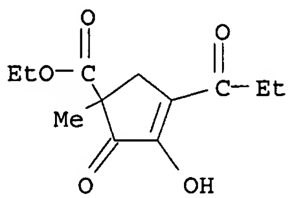
Absolute stereochemistry.



RN 26103-79-7 CAOLD
CN 3-Cyclopentene-1,3-dicarboxylic acid, 4-hydroxy-1-methyl-5-oxo-, diethyl ester (7CI, 9CI) (CA INDEX NAME)



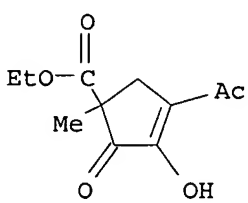
RN 92723-62-1 CAOLD
CN 3-Cyclopentene-1-carboxylic acid, 3-hydroxy-1-methyl-2-oxo-4-propionyl-, ethyl ester (7CI) (CA INDEX NAME)



RN 96380-22-2 CAOLD
CN 3-Cyclopentene-1-carboxylic acid, 4-acetyl-3-hydroxy-1-methyl-2-oxo-, ethyl ester, semicarbazone (7CI) (CA INDEX NAME)

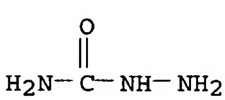
CM 1

CRN 780-73-4
CMF C11 H14 O5



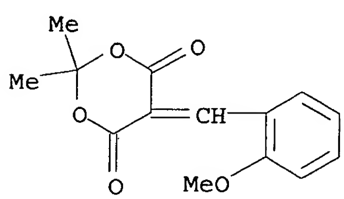
CM 2

CRN 57-56-7
CMF C H5 N3 O

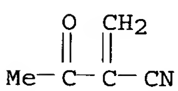


IT **78-94-4** **183-97-1** **759-65-9**
765-70-8 **769-45-9** **769-46-0**
771-74-4 778-06-3 780-73-4 783-70-0 786-14-1
889-67-8 26103-79-7 91062-15-6 92723-62-1 94520-21-5
96080-97-6 96380-22-2

L111 ANSWER 6 OF 21 CAOLD
ACCESSION NUMBER: CA61:7827h CAOLD
TITLE: least-sqs. local-energy method for mol.-energy level calcn.
AUTHOR NAME: Frost, Arthur A.
INDEX TERM: 922-64-5 1214-54-6 2826-28-0 4335-90-4 5381-33-9 15795-54-7 **15795-56-9** 15795-57-0 15875-48-6 15875-49-7 17474-27-0 20444-83-1 20444-87-5 **22163-77-5** 23111-03-7 23340-25-2 23340-26-3 26187-43-9 68588-31-8 90536-56-4 91688-54-9 94546-37-9 95218-82-9
IT **15795-56-9 22163-77-5**
RN 15795-56-9 CAOLD
CN 1,3-Dioxane-4,6-dione, 5-[(2-methoxyphenyl)methylene]-2,2-dimethyl- (9CI) (CA INDEX NAME)



RN 22163-77-5 CAOLD
CN Butanenitrile, 2-methylene-3-oxo- (9CI) (CA INDEX NAME)



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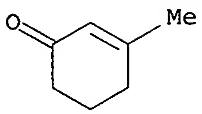
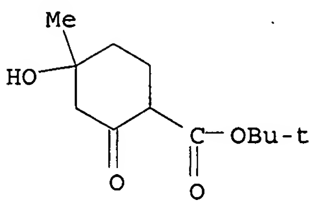
5381-33-9 15795-54-7 15795-56-9 15795-57-0 15875-48-6
15875-49-7 17474-27-0 20444-83-1 20444-87-5 22163-77-5
23111-03-7 23340-25-2 23340-26-3 26187-43-9 68588-31-8
90536-56-4 91688-54-9 94546-37-9 95218-82-9

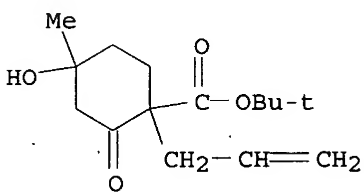
L111 ANSWER 7 OF 21 CAOLD
ACCESSION NUMBER: CA61:7047h CAOLD
TITLE: elimination - (VII) syntheses of DL-piperitone (DL-p-menthen-3-one) and related compds. from tert-butyl β-oxo esters
AUTHOR NAME: Lawesson, Sven O.; Larsen, E. H.; Jakobsen, H. J.; Frisell, C.
INDEX TERM: **1193-18-6 93043-68-6 94092-64-5 94428-39-4**
IT **1193-18-6 93043-68-6 94092-64-5 94428-39-4**
RN 1193-18-6 CAOLD
CN 2-Cyclohexen-1-one, 3-methyl- (7CI, 8CI, 9CI) (CA INDEX NAME)



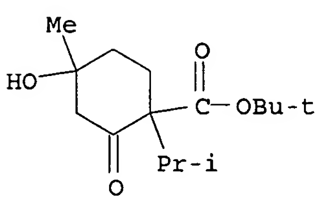
RN 93043-68-6 CAOLD
CN Cyclohexanecarboxylic acid, 4-hydroxy-4-methyl-2-oxo-, tert-butyl ester (7CI) (CA INDEX NAME)



RN 94092-64-5 CAOLD
CN Cyclohexanecarboxylic acid, 1-allyl-4-hydroxy-4-methyl-2-oxo-, tert-butyl ester (7CI) (CA INDEX NAME)



RN 94428-39-4 CAOLD
CN p-Menthane-4-carboxylic acid, 1-hydroxy-3-oxo-, tert-butyl ester (7CI) (CA INDEX NAME)

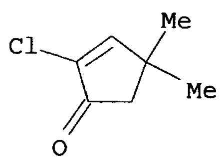


IT **1193-18-6** **93043-68-6** **94092-64-5**
94428-39-4

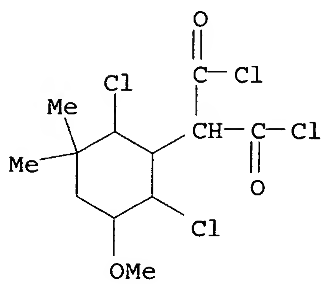
L111 ANSWER 8 OF 21 CAOLD COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: CA60:7926c CAOLD
TITLE: halogen-substituted 1,3-cyclohexanediones - (I) reaction of 2,2-dichlorodimedon with bases, (II) chlorinated cycloalkanones from 2,2-dichlorodimedon
AUTHOR NAME: Schamp, N.; Verzele, M.
INDEX TERM: 932-23-0 7298-86-4 10545-47-8 17257-68-0
17530-72-2 17530-74-4 17530-75-5

17554-69-7 17554-71-1 17554-72-2
17554-73-3 17554-76-6 17554-77-7 17554-78-8
17554-86-8 17554-87-9 90153-71-2
90560-70-6 93718-10-6

IT **17554-69-7** **90560-70-6**
RN 17554-69-7 CAOLD
CN 2-Cyclopenten-1-one, 2-chloro-4,4-dimethyl- (7CI, 8CI, 9CI) (CA INDEX NAME)

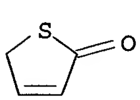


RN 90560-70-6 CAOLD
CN Cyclohexanemalonyl chloride, 2,6-dichloro-3-methoxy-5,5-dimethyl- (7CI) (CA INDEX NAME)

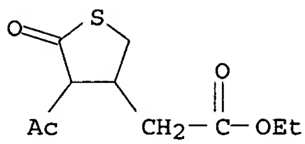


IT **932-23-0** **7298-86-4** 10545-47-8 17257-68-0
17530-72-2 17530-74-4 17530-75-5 17554-69-7 17554-71-1
17554-72-2 17554-73-3 17554-76-6 17554-77-7 17554-78-8
17554-86-8 17554-87-9 90153-71-2 90560-70-6 93718-10-6

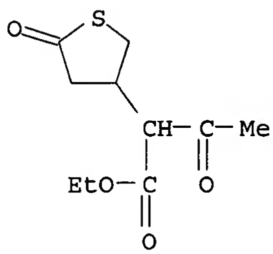
L111 ANSWER 9 OF 21 CAOLD COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: CA59:12740c CAOLD
TITLE: thiophene chemistry - (VIII) Michael addns. to 2(5H)-thiophenone
AUTHOR NAME: Jakobsen, Hans J.; Larsen, E. H.; Lawesson, S. O.
INDEX TERM: **3354-32-3** **94520-69-1** **98840-40-5**
IT **3354-32-3** **94520-69-1** **98840-40-5**
RN 3354-32-3 CAOLD
CN 2(5H)-Thiophenone (8CI, 9CI) (CA INDEX NAME)



RN 94520-69-1 CAOLD
CN Glutaric acid, 2-acetyl-3-(mercaptomethyl)-, 1-ethyl ester, γ-(thiolactone) (7CI) (CA INDEX NAME)

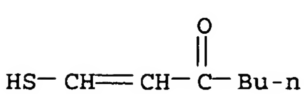


RN 98840-40-5 CAOLD
CN 3-Thiopheneacetic acid, α-acetyltetrahydro-5-oxo-, ethyl ester (7CI) (CA INDEX NAME)

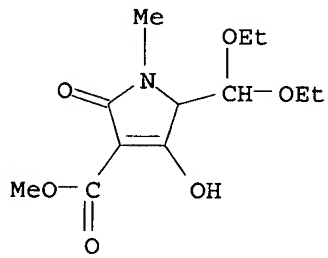


IT **3354-32-3** **94520-69-1** **98840-40-5**

L111 ANSWER 10 OF 21 CAOLD COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: CA59:6374h CAOLD
TITLE: total synthesis of the antibiotics thiolutin and holomycin
AUTHOR NAME: Schmidt, Ulrich; Geiger, F.
INDEX TERM: 87-11-6 488-04-0 17771-36-7 17771-37-8
17771-38-9 17958-78-0 40647-81-2 40970-25-0
40970-28-3 40970-29-4 61040-21-9 82031-42-3
86247-90-7 89531-66-8 **89896-91-3**
90345-39-4 90438-00-9 90612-05-8 90770-46-0
91013-69-3 91558-95-1 91807-18-0 92369-67-0
92576-32-4 92851-68-8 **93041-65-7**
93139-36-7 93262-81-8 93427-67-9 93689-26-0
94000-31-4 94488-37-6 94501-89-0 94584-10-8
95591-82-5 95875-90-4 95937-27-2 96775-79-0
96792-79-9 96951-63-2 97236-85-6 97525-12-7
97525-48-9 98000-64-7 98529-76-1 100152-96-3
106599-90-0
IT **89896-91-3** **93041-65-7**
RN 89896-91-3 CAOLD
CN 1-Hepten-3-one, 1-mercapto- (7CI) (CA INDEX NAME)



RN 93041-65-7 CAOLD
CN 3-Pyrroline-3-carboxylic acid, 5-formyl-4-hydroxy-1-methyl-2-oxo-, methyl ester, diethyl acetal (7CI) (CA INDEX NAME)



IT 87-11-6 488-04-0 17771-36-7 17771-37-8
17771-38-9 17958-78-0 40647-81-2 40970-25-0 40970-28-3
40970-29-4 61040-21-9 82031-42-3 86247-90-7 89531-66-8
89896-91-3 90345-39-4 90438-00-9 90612-05-8 90770-46-0
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95591-82-5 95875-90-4 95937-27-2 96775-79-0 96792-79-9
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98529-76-1 100152-96-3 106599-90-0

L111 ANSWER 11 OF 21 CAOLD
ACCESSION NUMBER: CA59:585b CAOLD
TITLE: condensation reactions with isoxazoles-extension of the Ritter reaction
AUTHOR NAME: Eugster, Conrad H.; Leichner, L.; Jenny, E.
INDEX TERM: 3949-36-8 6317-31-3 17433-51-1
18938-02-8 23340-25-2 33185-16-9 42222-06-0
43135-05-3 57524-14-8 63879-04-9 72152-84-2
73661-48-0 78450-21-2 78450-22-3 88590-04-9
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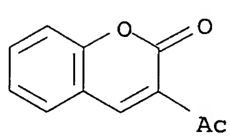
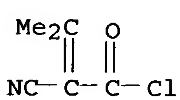
90565-41-6 90978-55-5 91137-31-4 91240-33-4
91251-51-3 91251-95-5 91252-52-7 91253-23-5
91253-30-4 91333-88-9 91718-35-3 92027-20-8
92151-50-3 92188-50-6 92244-26-3 92646-74-7
92652-35-2
IT 3949-36-8 89379-78-2
RN 3949-36-8 CAOLD
CN 2H-1-Benzopyran-2-one, 3-acetyl- (9CI) (CA INDEX NAME)



RN 89379-78-2 CAOLD
CN Crotonoyl chloride, 2-cyano-3-methyl- (6CI, 7CI) (CA INDEX NAME)



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91252-52-7	91253-23-5	91253-30-4	91333-88-9	91718-35-3
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92652-35-2				

L111 ANSWER 12 OF 21 CAOLD
ACCESSION NUMBER: CA58:9420e CAOLD
TITLE: effects of chemicals on the mitotic cell in plant-tropoids
AUTHOR NAME: Shimizu, Yoshitaka
INDEX TERM:

363-67-7	641-28-1	**698-18-0**	
1210-27-1	2132-33-4	2161-21-9	2161-40-2
2161-45-7	2229-97-2	2745-10-0	3331-45-1
3336-70-7	3336-74-1	3480-08-8	3525-04-0
3525-06-2	3525-13-1	3806-02-8	
3839-48-3	4481-35-0	**6264-93-3**	
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23957-64-4	25946-69-4	27571-10-4	33739-56-9
33756-57-9	33902-86-2	**36039-41-5**	
36044-38-9	50472-20-3	50472-24-7	51163-64-5
67931-57-1	86371-89-3	88614-27-1	88614-51-1
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92819-49-3	92847-26-2	92850-76-5	
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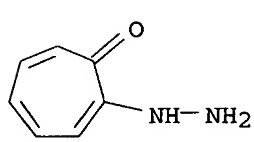
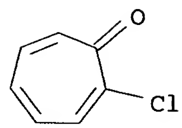
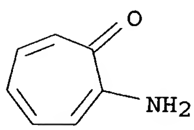
IT **698-18-0** **3839-48-3** **6264-93-3**
36039-41-5 **89975-62-2** **92959-86-9**
RN 698-18-0 CAOLD
CN 2,4,6-Cycloheptatrien-1-one, 2-hydrazino- (7CI, 8CI, 9CI) (CA INDEX NAME)



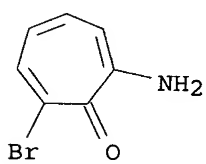
RN 3839-48-3 CAOLD
CN 2,4,6-Cycloheptatrien-1-one, 2-chloro- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



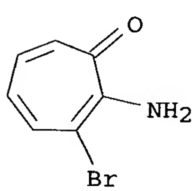
RN 6264-93-3 CAOLD
CN 2,4,6-Cycloheptatrien-1-one, 2-amino- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



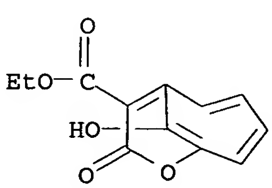
RN 36039-41-5 CAOLD
CN 2,4,6-Cycloheptatrien-1-one, 2-amino-7-bromo- (7CI, 9CI) (CA INDEX NAME)



RN 89975-62-2 CAOLD
CN 2,4,6-Cycloheptatrien-1-one, 2-amino-3-bromo- (6CI, 7CI) (CA INDEX NAME)



RN 92959-86-9 CAOLD
CN 2,4,6-Cycloheptatriene-Δ1,α-malonic acid, 2,3-dihydroxy-, δ-lactone, ethyl ester (7CI) (CA INDEX NAME)



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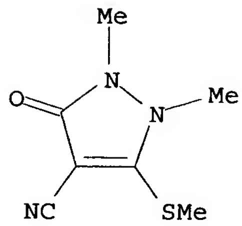
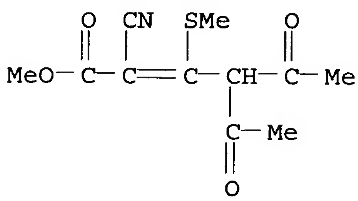
86371-89-3 88614-27-1 88614-51-1 89583-83-5 89975-62-2
89976-57-8 90005-81-5 90035-67-9 90326-38-8 90557-54-3
90560-17-1 90560-38-6 90766-32-8 90770-92-6 90887-13-1
90914-87-7 90922-80-8 91091-48-4 91805-09-3 91820-16-5
91955-17-8 91983-38-9 91997-34-1 91997-52-3 92026-81-8
92248-31-2 92254-30-3 92288-77-2 92381-56-1 92765-09-8
92819-49-3 92847-26-2 92850-76-5 92959-86-9 93008-66-3
93011-82-6 93187-11-2 93353-13-0 93738-09-1 93817-25-5
94269-56-4 94296-56-7 94303-45-4 94378-21-9 94488-35-4
94673-71-9 94997-50-9 95140-61-7 95163-70-5 95767-12-7
95767-13-8 97980-17-1 98494-99-6 100196-33-6 100232-84-6
102924-42-5 104879-21-2

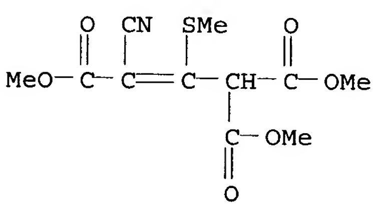
L111 ANSWER 13 OF 21 CAOLD COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: CA58:9067c CAOLD
TITLE: carboxylic acid derivs. - (V) ketene derivs. (I) substituted dithiocarboxylic acids and ketene mercaptals, (II) reactions of substituted ketene mercaptals, (III) pyrazoles and isoxazoles from ketene mercaptals
AUTHOR NAME: Gompper, Rudolf; Toepfl, W.
INDEX TERM: 2080-43-5 2276-43-9 2939-72-2 3490-92-4
4933-40-8 5147-80-8 5624-24-8 10354-92-4
10355-19-8 17823-64-2 17823-65-3 17823-69-7
18071-20-0 19607-08-0 23858-31-3 25241-08-1
25241-12-7 29866-36-2 29866-38-4 37614-61-2
37758-35-3 51531-96-5 51532-03-7 52046-75-0
52793-49-4 59334-11-1 60312-08-5 63114-05-6
68313-63-3 72760-85-1 81385-18-4 85106-72-5
88550-49-6 88614-56-6 89489-55-4
89853-59-8 90434-81-4 90771-90-7
90842-90-3 90916-95-3 91058-84-3
91134-34-8 **91134-83-7** 91807-27-1
91912-29-7 91974-70-8 92289-68-4 92548-31-7
92723-91-6 92801-12-2 **92964-02-8**
93013-94-6 94031-91-1 94066-35-0 94267-21-7
94933-83-2 **94982-52-2** 95533-91-8
95697-30-6 96329-56-5 97103-00-9 97299-68-8
97441-93-5 97595-95-4 97595-96-5 97725-92-3
97980-57-9 99996-85-7 100168-89-6
IT **89853-59-8** **91134-34-8** **91134-83-7**
92964-02-8 **94982-52-2**
RN 89853-59-8 CAOLD
CN 3-Pyrazoline-4-carbonitrile, 1,2-dimethyl-3-(methylthio)-5-oxo- (7CI) (CA INDEX NAME)



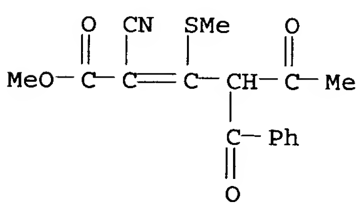
RN 91134-34-8 CAOLD
CN 2-Hexenoic acid, 4-acetyl-2-cyano-3-(methylthio)-5-oxo-, methyl ester (7CI) (CA INDEX NAME)



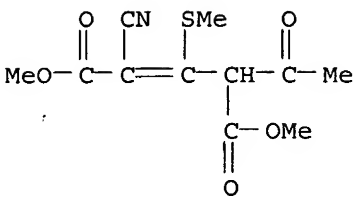
RN 91134-83-7 CAOLD
CN 2-Propene-1,1,3-tricarboxylic acid, 3-cyano-2-(methylthio)-, trimethyl ester (7CI) (CA INDEX NAME)



RN 92964-02-8 CAOLD
CN 2-Hexenoic acid, 4-benzoyl-2-cyano-3-(methylthio)-5-oxo-, methyl ester (7CI) (CA INDEX NAME)



RN 94982-52-2 CAOLD
CN Glutaconic acid, 4-acetyl-2-cyano-3-(methylthio)-, dimethyl ester (7CI) (CA INDEX NAME)



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3490-92-4 **4933-40-8** 5147-80-8 5624-24-8
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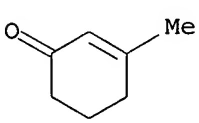
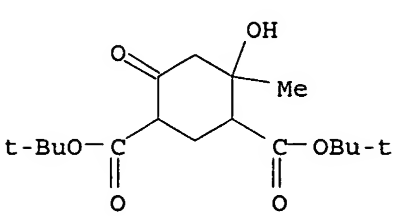
29866-36-2 29866-38-4 37614-61-2 37758-35-3 51531-96-5
51532-03-7 52046-75-0 52793-49-4 59334-11-1 60312-08-5
63114-05-6 68313-63-3 72760-85-1 81385-18-4 85106-72-5
88550-49-6 88614-56-6 89489-55-4 89853-59-8 90434-81-4
90771-90-7 90842-90-3 90916-95-3 91058-84-3 91134-34-8
91134-83-7 91807-27-1 91912-29-7 91974-70-8 92289-68-4
92548-31-7 92723-91-6 92801-12-2 92964-02-8 93013-94-6
94031-91-1 94066-35-0 94267-21-7 94933-83-2 94982-52-2
95533-91-8 95697-30-6 96329-56-5 97103-00-9 97299-68-8
97441-93-5 97595-95-4 97595-96-5 97725-92-3 97980-57-9
99996-85-7 100168-89-6

L111 ANSWER 14 OF 21 CAOLD COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: CA58:5529a CAOLD
TITLE: elimination - (V) synthesis of 1-methyl-1-cyclohexen-3-one and related compds.
AUTHOR NAME: Naslund, Gunnel; Senning, A.; Lawesson, S. O.
INDEX TERM: **1193-18-6** 5715-25-3 94329-15-4
94801-98-6 95169-78-1 95557-23-6
96171-90-3 96268-73-4
IT **1193-18-6** **94801-98-6**
RN 1193-18-6 CAOLD
CN 2-Cyclohexen-1-one, 3-methyl- (7CI, 8CI, 9CI) (CA INDEX NAME)



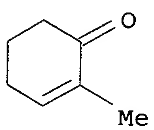
RN 94801-98-6 CAOLD
CN 1,3-Cyclohexanedicarboxylic acid, 4-hydroxy-4-methyl-6-oxo-, di-tert-butyl ester (7CI) (CA INDEX NAME)



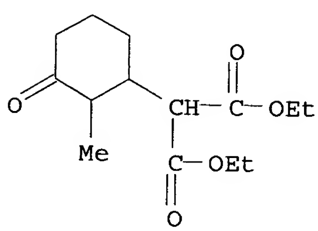
IT **1193-18-6** **5715-25-3** 94329-15-4 94801-98-6

95169-78-1 95557-23-6 96171-90-3 96268-73-4

L111 ANSWER 15 OF 21 CAOLD COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: CA56:9998g CAOLD
TITLE: synthesis of terpenes - (VII) 9-methyl-6-oxo-Δ4(10)-1-octahydro-naphthyleneacetic acid
AUTHOR NAME: Davis, Brian Reeve; Gupta, S. R.; Halsall, T. G.
INDEX TERM: **1121-18-2** **6272-53-3**
37457-15-1 57026-73-0 65093-74-5 90975-34-1
91966-06-2 92730-34-2 93726-57-9 94092-45-2
95556-08-4 97261-87-5
IT **1121-18-2** **6272-53-3**
RN 1121-18-2 CAOLD
CN 2-Cyclohexen-1-one, 2-methyl- (7CI, 8CI, 9CI) (CA INDEX NAME)



RN 6272-53-3 CAOLD
CN Propanedioic acid, (2-methyl-3-oxocyclohexyl)-, diethyl ester (9CI) (CA INDEX NAME)



IT **1121-18-2** **6272-53-3** 37457-15-1 57026-73-0
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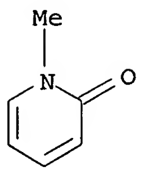
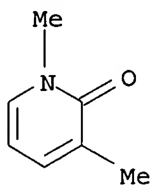
94092-45-2 95556-08-4 97261-87-5

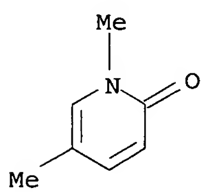
L111 ANSWER 16 OF 21 CAOLD COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: CA55:19918d CAOLD
TITLE: aromaticity by nuclear resonance spectroscopy - (I) 2-pyridones and related systems
AUTHOR NAME: Elvidge, J. A.; Jackman, L. M.
INDEX TERM: 689-89-4 **694-85-9** 1003-56-1
1149-24-2 1150-55-6 **6456-92-4**
6456-93-5 **15031-43-3** 15031-89-7
15827-70-0 22739-24-8 31349-63-0 39594-85-9
100610-52-4 109103-38-0 111063-62-8
132778-74-6
IT **694-85-9** **6456-92-4** **6456-93-5**
15031-43-3 **100610-52-4**
RN 694-85-9 CAOLD
CN 2(1H)-Pyridinone, 1-methyl- (9CI) (CA INDEX NAME)



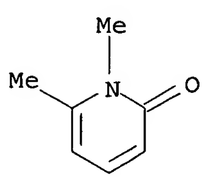
RN 6456-92-4 CAOLD
CN 2(1H)-Pyridinone, 1,3-dimethyl- (9CI) (CA INDEX NAME)



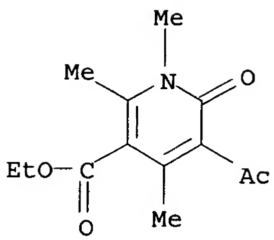
RN 6456-93-5 CAOLD
CN 2(1H)-Pyridinone, 1,5-dimethyl- (9CI) (CA INDEX NAME)



RN 15031-43-3 CAOLD
CN 2(1H)-Pyridinone, 1,6-dimethyl- (9CI) (CA INDEX NAME)



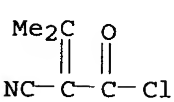
RN 100610-52-4 CAOLD
CN Nicotinic acid, 5-acetyl-1,6-dihydro-1,2,4-trimethyl-6-oxo-, ethyl ester (6CI) (CA INDEX NAME)



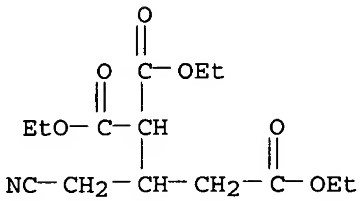
IT **689-89-4** **694-85-9** **1003-56-1**
1149-24-2 **1150-55-6** 6456-92-4 6456-93-5
15031-43-3 15031-89-7 15827-70-0 22739-24-8 31349-63-0
39594-85-9 100610-52-4 109103-38-0 111063-62-8 132778-74-6

L111 ANSWER 17 OF 21 CAOLD
ACCESSION NUMBER: CA53:332a CAOLD
TITLE: active components of Digenea simplex and related compds. - (LIV) synthesis of 2-carboxy-3-pyrrolidineacetic acid (2-i), (LV) (2-ii), (LVI) of L-α-dihydrokainic acid (2-i), (LVII) (2-ii), (LVIII) of L-α-allokainic acid (3)
AUTHOR NAME: Sugawa, Toshio
INDEX TERM: 759-21-7 3731-16-6 10444-38-9 14869-34-2
17216-62-5 49785-86-6 58474-93-4
89379-78-2 89775-98-4 90979-03-6
93273-12-2 **93432-60-1** 96229-51-5
97497-60-4 98133-48-3 98140-80-8 98491-69-1
98547-29-6 99075-65-7 99076-43-4 99076-47-8
99176-40-6 99189-77-2 100132-48-7 100453-82-5
101020-91-1 101086-73-1 **101086-74-2**
101109-05-1 101568-82-5 101589-43-9 101777-53-1
101867-55-4 102015-01-0 102074-21-5 102708-95-2
102878-66-0 104743-70-6 104912-63-2 106163-77-3
106275-34-7 **107777-89-9** 107923-09-1
108085-38-7 **108479-31-8** 109162-12-1
109731-65-9 111007-80-8 112441-11-9 117343-07-4
119417-53-7 131241-49-1

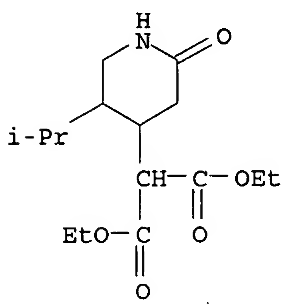
IT **89379-78-2** **93432-60-1** **101086-74-2**
107777-89-9 **108479-31-8**
RN 89379-78-2 CAOLD
CN Crotonoyl chloride, 2-cyano-3-methyl- (6CI, 7CI) (CA INDEX NAME)



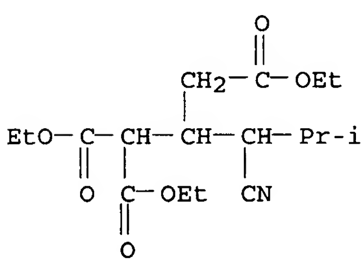
RN 93432-60-1 CAOLD
CN 1,1,3-Propanetricarboxylic acid, 2-(cyanomethyl)-, triethyl ester (6CI, 7CI) (CA INDEX NAME)



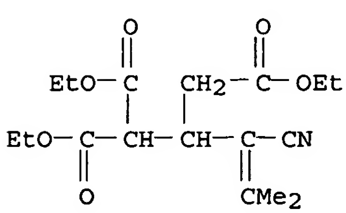
RN 101086-74-2 CAOLD
CN 4-Piperidinemalonic acid, 5-isopropyl-2-oxo-, diethyl ester (6CI) (CA INDEX NAME)



RN 107777-89-9 CAOLD
CN 1,1,3-Propanetricarboxylic acid, 2-(1-cyano-2-methylpropyl)-, triethyl ester (6CI) (CA INDEX NAME)



RN 108479-31-8 CAOLD
CN 1,1,3-Propanetricarboxylic acid, 2-(1-cyano-2-methylpropenyl)-, triethyl ester (6CI) (CA INDEX NAME)



IT **759-21-7** **3731-16-6** **10444-38-9**
14869-34-2 **17216-62-5** 49785-86-6 58474-93-4

89379-78-2 89775-98-4 90979-03-6 93273-12-2 93432-60-1
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101867-55-4 102015-01-0 102074-21-5 102708-95-2 102878-66-0
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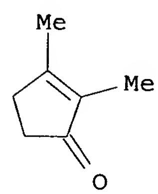
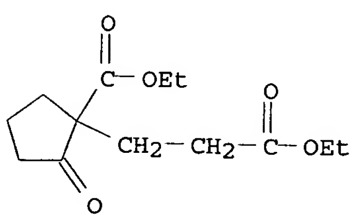
107923-09-1 108085-38-7 108479-31-8 109162-12-1 109731-65-9
111007-80-8 112441-11-9 117343-07-4 119417-53-7 131241-49-1

L111 ANSWER 18 OF 21 CAOLD
ACCESSION NUMBER: CA52:2848h CAOLD
TITLE: organic reactions with polyphosphoric acid - (V) intramol. acylation with lactones-cyclopentenones from α-lactones
AUTHOR NAME: Dev, Sukh; Rai, C.
INDEX TERM: **1121-05-7** 1572-39-0 1572-40-3
2275-26-5 3296-45-5 4430-31-3 6053-92-5
6818-07-1 10413-18-0 22117-99-3 22118-00-9
57026-64-9 84196-94-1 89244-93-9
93865-05-5 110061-30-8 116154-62-2

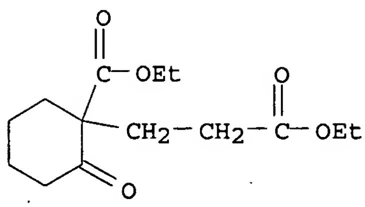
IT **1121-05-7** **57026-64-9** **93865-05-5**
RN 1121-05-7 CAOLD
CN 2-Cyclopenten-1-one, 2,3-dimethyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



RN 57026-64-9 CAOLD
CN Cyclopentanepropanoic acid, 1-(ethoxycarbonyl)-2-oxo-, ethyl ester (9CI) (CA INDEX NAME)



RN 93865-05-5 CAOLD
CN Cyclohexanepropanoic acid, 1-(ethoxycarbonyl)-2-oxo-, ethyl ester (9CI) (CA INDEX NAME)



IT **1121-05-7** **1572-39-0** **1572-40-3**
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10413-18-0 22117-99-3 22118-00-9 57026-64-9 84196-94-1
89244-93-9 93865-05-5 110061-30-8 116154-62-2

L111 ANSWER 19 OF 21 CAOLD

ACCESSION NUMBER: CA51:15699h CAOLD
TITLE: synthetic compds. active against Salmonella dysentery group bacilli
AUTHOR NAME: Akiya, Shichiro
INDEX TERM:

83-72-7	90-46-0	92-83-1	94-77-9
100-56-1	120-11-6	121-52-8	230-27-3
300-25-4	304-91-6	479-22-1	518-75-2
532-96-7	604-44-4	616-82-0	619-14-7
626-03-9	633-65-8	669-95-4	683-57-8
699-18-3	710-25-8	831-71-0	1010-60-2
1013-10-1	1083-30-3	1088-95-5	1090-16-0
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6699-22-5	7152-80-9	7208-14-2	7341-60-8
7355-34-2	7410-54-0	**7460-87-9**	
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24305-56-4	24305-58-6	24313-95-9	24849-77-2
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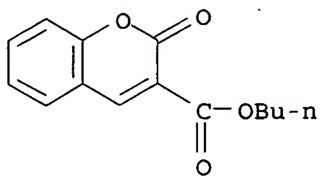
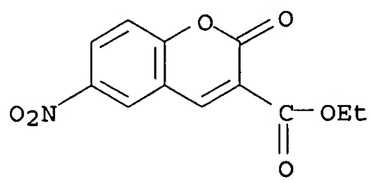
101090-86-2 116890-40-5 117756-51-1

RN 7460-87-9 CAOLD

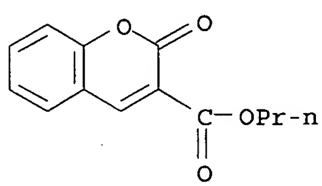
CN 2H-1-Benzopyran-3-carboxylic acid, 2-oxo-, butyl ester (6CI, 9CI) (CA INDEX NAME)



RN 13373-28-9 CAOLD
CN 2H-1-Benzopyran-3-carboxylic acid, 6-nitro-2-oxo-, ethyl ester (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



RN 39497-12-6 CAOLD
CN 2H-1-Benzopyran-3-carboxylic acid, 2-oxo-, propyl ester (6CI, 9CI) (CA INDEX NAME)



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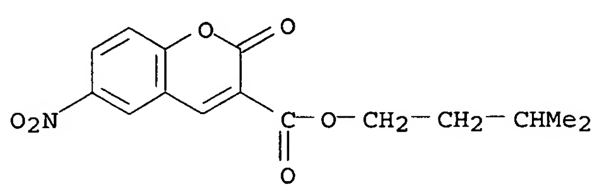

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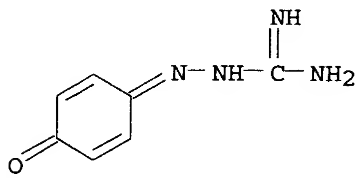
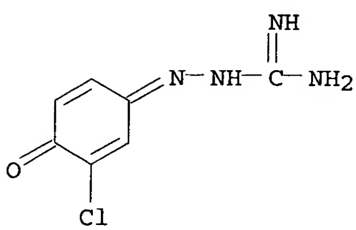
CN Guanidine, [(dichloro-4-oxo-2,5-cyclohexadien-1-ylidene)amino]- (6CI) (CA INDEX NAME)



2 (D1—Cl)

RN 117756-51-1 CAOLD
CN Guanidine, [(3-chloro-4-oxo-2,5-cyclohexadien-1-ylidene)amino]-
(6CI) (CA INDEX NAME)



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L111 ANSWER 20 OF 21 CAOLD COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: CA51:12890c CAOLD

TITLE: reaction of β-chlorovinyl ketones with β-dicarbonyl compds. - (III) ketovinylation of malonic ester-new synthesis of α-pyrones

AUTHOR NAME: Kochetkov, N. K.; Kudryashov, L. I.

INDEX TERM: 105-32-8 105-53-3 3306-07-8 **6465-10-7 6465-13-0 6465-14-1 7119-27-9 15787-72-1 99186-81-9 100059-41-4 100521-51-5 100533-49-1**

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100533-49-1

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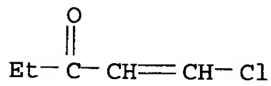

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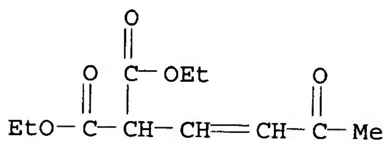
CN Propanedioic acid, (3-oxo-1-butenyl)-, diethyl ester (9CI) (CA INDEX NAME)



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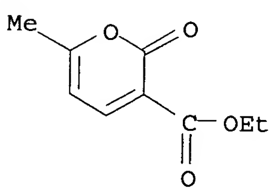

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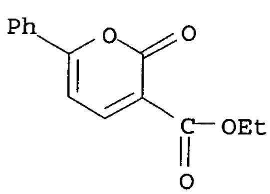

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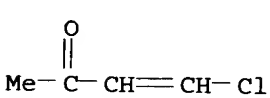
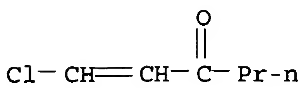


RN 15787-72-1 CAOLD

CN 1-Hexen-3-one, 1-chloro- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



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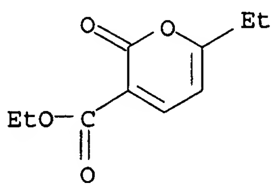

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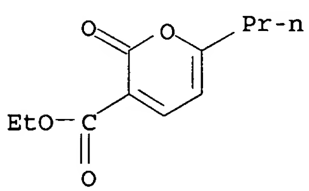

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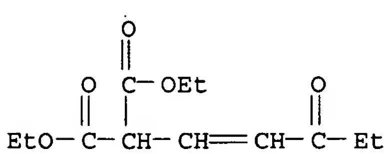

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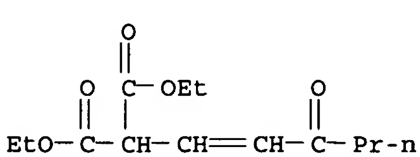

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L111 ANSWER 21 OF 21 CAOLD
ACCESSION NUMBER: CA51:4439a CAOLD
TITLE: 5-[2-(and 3)oxoalkyl]-2-thiohydantoins
AUTHOR NAME: Archer, Sydney
PATENT ASSIGNEE: Sterling Drug Inc.
DOCUMENT TYPE: Patent

PATENT NO.	KIND	DATE
PI US 2763662		1956

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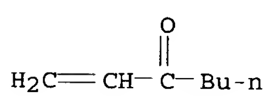

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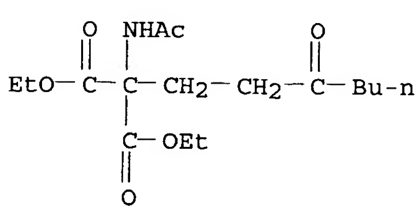

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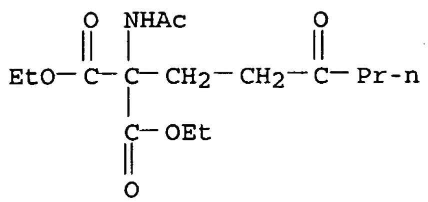

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103396-17-4 104116-05-4 104116-51-0 107306-09-2 109439-06-7
116080-78-5

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=> => d que stat l99
L97                QUE  ABB=ON  PLU=ON  (KANTO(W)KAGAKU?)/PA,CS,CO,SO
L98                QUE  ABB=ON  PLU=ON  WATANABE M?/AU OR MURATA K?/AU OR
                   IKARIYA T?/AU
L99             12 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L97 AND L98


=> d que stat l104
L97                QUE  ABB=ON  PLU=ON  (KANTO(W)KAGAKU?)/PA,CS,CO,SO
L98                QUE  ABB=ON  PLU=ON  WATANABE M?/AU OR MURATA K?/AU OR
                   IKARIYA T?/AU
L104            18 SEA L97 AND L98


=> d que stat l105
L97                QUE  ABB=ON  PLU=ON  (KANTO(W)KAGAKU?)/PA,CS,CO,SO
L98                QUE  ABB=ON  PLU=ON  WATANABE M?/AU OR MURATA K?/AU OR
                   IKARIYA T?/AU
L99             12 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L97 AND L98
L104            18 SEA L97 AND L98
L105            18 DUP REM L99 L104 (12 DUPLICATES REMOVED)


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YOU HAVE REQUESTED DATA FROM FILE 'HCAPLUS, WPIX' - CONTINUE? (Y)/N:y
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L105 ANSWER 1 OF 18 HCAPLUS COPYRIGHT 2006 ACS on STN DUPLICATE 1
ACCESSION NUMBER: 2005:207662 HCAPLUS
DOCUMENT NUMBER: 142:297886
TITLE: Process for preparing optically active nitro compounds and cyano compounds
INVENTOR(S): **Watanabe, Masahito; Murata, Kunihiko; Ikariya, Takao**
PATENT ASSIGNEE(S): **Kanto Kagaku** Kabushiki Kaisha, Japan
SOURCE: Eur. Pat. Appl., 35 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1512678	A1	20050309	EP 2004-20962	20040903
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, HR				
JP 2005187446	A2	20050714	JP 2004-76663	20040317
US 2005101787	A1	20050512	US 2004-934338	20040903

CN 1626501	A	20050615	CN 2004-10068730	2004 0906
PRIORITY APPLN. INFO.:			JP 2003-314096 A	2003 0905
			JP 2003-407981 A	2003 1205
			JP 2004-76663 A	2004 0317

OTHER SOURCE(S): CASREACT 142:297886; MARPAT 142:297886

ED Entered STN: 09 Mar 2005

AB Optically active nitro and cyano compds. (I) [wherein R1 = each (un)substituted aromatic mono- or polycyclic hydrocarbon, (un)saturated aliphatic or alicyclic hydrocarbon, hetero-mono- or polycyclic group, H, halogen, CO2H or its ester or amido, HO, alkoxy, NH2; R2, R3 = H, each (un)substituted aromatic mono- or polycyclic hydrocarbon, (un)saturated aliphatic or alicyclic hydrocarbon, or hetero-mono- or polycyclic group; X = NO2, cyano; or two of R1-R3 can form a ring binding each other; R4 = H, halogen, amido, amino, alkoxy, NO2, cyano, each (un)substituted aromatic mono- or polycyclic hydrocarbon, (un)saturated aliphatic or alicyclic hydrocarbon, or hetero-mono- or polycyclic group; R5, R6 = H, each (un)substituted aromatic mono- or polycyclic hydrocarbon, or (un)saturated aliphatic or alicyclic hydrocarbon group, straight or branched C1-20 alkoxy; oe two of R4-R6 can form a ring binding each other; Y, Z = a single bond, O, S, N, P; m, n = 1, 2; in the case that Y and Z are a single bond, O or S atom, m and n are 1, and in the case that Y and Z are N or P atom, m and n are 2] are prepared in high efficiency and high stereoselectivity by simple and practical asym. Michael reaction of nitroethene or acrylonitrile derivs. (II) with dialkyl malonates or acylacetates (III) in the presence of a chiral metal complex, which is obtained by reaction of an optically active nitrogen-containing compound and a periodic table group VIII metal complex. Thus, [(S,S)-N-(2,4,6-triisopropylbenzenesulfonyl)-1,2-diphenylethylenediamine](hexamethylbenzene)ruthenium (14.8 mg, 0.02 mmol, S/C = 50), trans-p-nitrostyrene (149 mg, 1.0 mmol), di-Me malonate (114 μL, 1.0 mmol) and toluene (1 mL) were added into a Schlenk tube (20 mL) under an argon atmospheric, and stirred at 30° for 24 h to give, after purification by flash column chromatog. (hexane/acetone = 80/20, SiO2), 94% Me (R)-2-methoxycarbonyl-4-nitro-3-phenylbutanoate (87% ee).

IC ICM C07C255-22
ICS C07C205-53

CC 25-20 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
Section cross-reference(s): 27, 29

REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L105 ANSWER 2 OF 18 HCAPLUS COPYRIGHT 2006 ACS on STN DUPLICATE 2

ACCESSION NUMBER: 2004:584477 HCAPLUS

DOCUMENT NUMBER: 141:140101

TITLE: Process and catalysts for producing optically

active cycloalkylmalonates
INVENTOR(S): **Watanabe, Masahito; Murata, Kunihiko; Ikariya, Takao**
PATENT ASSIGNEE(S): **Kanto Kagaku** Kabushiki Kaisha, Japan
SOURCE: Eur. Pat. Appl., 29 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1439159	A1	20040721	EP 2004-296	20040109
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
JP 2004269481	A2	20040930	JP 2003-71368	20030317
US 2004176616	A1	20040909	US 2003-749806	20031231
PRIORITY APPLN. INFO.:			JP 2003-9786 A	20030117
			JP 2003-71368 A	20030317

OTHER SOURCE(S): MARPAT 141:140101
ED Entered STN: 22 Jul 2004
AB Optically active malonate derivs. R1COCR2R3CR4(COXR5)COYR6 [R1 = (un)substituted aromatic, aliphatic, alicyclic, heterocyclic, H, alkoxy, amino; R2-R4 = H, (un)substituted aryl, aliphatic, alicyclic, heterocyclic; R1R2, R1R3, R2R3, R4R5, R5R6, R4R6 = atoms required to form a ring; R5, R6 = H, (un)substituted aryl, aliphatic, alicyclic, alkoxy; X, Y = bond; XR5, YR6 = (un)substituted OH, NH2] were prepared by treating R1COCH:CR2R3 with R4CH(COXR5)COYR6 in presence of an asym. metal catalyst, preferably a Ru catalyst I [R7-R10 = (un)substituted Ph]. Thus, [RuCl2(C6Me6)]2 was treated with (S,S)-TsDPEN to give Ru[(S,S)-TsDPEN](C6Me6) which was used in the Michael reaction of 2-cyclohexenone with CH2(CO2Me)2 to give (R)-3-[bis(methoxycarbonyl)methyl]cyclohexanone in 96% ee.
IC ICM C07C045-72
CC 24-5 (Alicyclic Compounds)

L105 ANSWER 3 OF 18 HCAPLUS COPYRIGHT 2006 ACS on STN DUPLICATE 3
ACCESSION NUMBER: 2003:356091 HCAPLUS
DOCUMENT NUMBER: 138:353733
TITLE: Process for producing optically active amino alcohols
INVENTOR(S): **Watanabe, Masahito; Murata, Kunihiko; Ikariya, Takao**
PATENT ASSIGNEE(S): **Kanto Kagaku** Kabushiki

	Kaisha, Japan
SOURCE:	Eur. Pat. Appl., 23 pp. CODEN: EPXXDW
DOCUMENT TYPE:	Patent
LANGUAGE:	English
FAMILY ACC. NUM. COUNT:	1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
EP 1308435	A2	20030507	EP 2002-24517		20021030
EP 1308435	A3	20030604			
EP 1308435	B1	20051228			
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK					
JP 2003201269	A2	20030718	JP 2002-251994		20020829
JP 3504254	B2	20040308			
CA 2409906	AA	20030430	CA 2002-2409906		20021028
JP 2003201270	A2	20030718	JP 2002-316217		20021030
US 2003171592	A1	20030911	US 2002-285164		20021031
US 6686505	B2	20040203			
PRIORITY APPLN. INFO.:			JP 2001-335322	A	20011031
			JP 2002-251994	A	20020829

OTHER SOURCE(S): MARPAT 138:353733

ED Entered STN: 09 May 2003

AB A process for producing an optically active amino alc. is provided that includes a step in which a nitro ketone or a cyano ketone is reacted with a hydrogen-donating organic or inorg. compound in the presence of a transition metal compound catalyst having an optically active nitrogen-containing compound as an asym. ligand to give an optically active nitro alc. or an optically active cyano alc., and a step in which the above optically active alc. is further reduced to efficiently produce an optically active amino alc. Thus, PhCOCH2CN was reduced with HCO2H in presence of Et3N and chloro[(S,S)-N-(p-toluenesulfonyl)-1,2-diphenylethylenediamine](p-cymene)ruthenium to give (S)-HOCHPhCH2CN in 98% ee. This compound was reduced with BH3.Me2S to give (S)-HOCHPhCH2CH2NH2 with 98% ee. The alcs. are intermediates for pharmaceuticals, such as fluoxetine, tomoxetine, nisoxetine and norfluoxetine.

IC ICM C07C201-12
ICS C07C253-30; C07C213-02

CC 25-7 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)

Section cross-reference(s): 27

L105 ANSWER 4 OF 18 HCAPLUS COPYRIGHT 2006 ACS on STN DUPLICATE 4
ACCESSION NUMBER: 1999:683209 HCAPLUS
DOCUMENT NUMBER: 131:310940
TITLE: Preparation method of bridged metallocene compounds
INVENTOR(S): Hori, Junichi; **Murata, Kunihiko**; Yoshida, Masahiro
PATENT ASSIGNEE(S): **Kanto Kagaku** K. K., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 37 pp. CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 11292891	A2	19991026	JP 1998-107170	19980403
PRIORITY APPLN. INFO.:			JP 1998-107170	19980403

OTHER SOURCE(S): MARPAT 131:310940
ED Entered STN: 27 Oct 1999
AB Title compds., useful as catalysts for olefin polymerization or organic synthesis, are prepared by reaction of Group 4 transition metal compds. I and (M2)+(L1)-C(L2)-(M2)+ and are represented by the general formula II, where M1 = Group 4 transition metal; A = Group 15 or 16 heteroatom; B = Group 14 typical element; R1, R2 = (heteroatom-containing) C1-30 hydrocarbyl or H; X = halogen or O- or S-containing C1-10 group; p, q = 0, 1, or 2; p + q = 1 or 2; r = 1 or 2; s = 2 or 3; L1, L2 = (substituted) cyclopentadienyl, (substituted) indenyl, (substituted) azulenyl, or (substituted) fluorenyl; C = C1-20 hydrocarbyl, (C1-20 hydrocarbyl-containing) silylene, oligosilylene, or germirene; M2 = Group 1 or 2 typical metal; and t = s-2, etc. Halogenated metallocene compds. III (Y = halogen) are stereoselectively prepared from II. Thus, (N-methylanilide)zirconium trichloride bistetrahydrofuran was prepared from N-methylaniline, ZrCl4, and THF, and reacted with 1,2-bis(3-indenyl)ethane dilithium salt to give ethylenebis(1-indenyl)zirconium (N-methylanilide) chloride.
IC ICM C07F017-00
CC 35-3 (Chemistry of Synthetic High Polymers)
Section cross-reference(s): 29, 67

L105 ANSWER 5 OF 18 HCAPLUS COPYRIGHT 2006 ACS on STN DUPLICATE 5
ACCESSION NUMBER: 1999:680136 HCAPLUS
DOCUMENT NUMBER: 131:310939
TITLE: Organic transition metal chemical compound
INVENTOR(S): Hori, Junichi; **Murata, Kunihiko**; Yoshida, Masahiro
PATENT ASSIGNEE(S): **Kanto Kagaku** K. K., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 37 pp. CODEN: JKXXAF
DOCUMENT TYPE: Patent

LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 11292890	A2	19991026	JP 1998-107169	19980403
PRIORITY APPLN. INFO.:			JP 1998-107169	19980403

OTHER SOURCE(S): MARPAT 131:310939
ED Entered STN: 26 Oct 1999
AB The title compds. comprise I (M = group 4 metal; A = group 15 heteroatom; B = Si, Ge, Sn, Pb; R1 = H, C1-20 hydrocarbyl which may contain heteroatoms; R2 = H, C1-20 hydrocarbyl; X = halogen; p, q = 0-2, p + q = 2; r = 1, 2; s = 2, 3, etc.). (N-Methylanilide)zirconium trichloride was prepared from N-methylaniline and ZrCl4, then reacted with dimethylsilylene bis indene dilithium salt to give dimethylsilylene bis (1-indenyl) zirconium (N-methylanilide) chloride.
IC ICM C07F017-00
CC 35-3 (Chemistry of Synthetic High Polymers)
Section cross-reference(s): 29, 67

L105 ANSWER 6 OF 18 HCAPLUS COPYRIGHT 2006 ACS on STN DUPLICATE 6
ACCESSION NUMBER: 1999:431903 HCAPLUS
DOCUMENT NUMBER: 131:87713
TITLE: Preparation of ruthenium-phosphine-amine complexes and stereoselective hydrogenation of carbonyl compounds to optically active alcohols using the complexes
INVENTOR(S): **Ikariya, Takao**; Ikehira, Hideyuki; **Murata, Kunihiko**; Kiyofuji, Nobuo; Ooka, Koji; Hashiguchi, Shohei; Okuma, Takeshi; Noyori, Ryoji
PATENT ASSIGNEE(S): Foundation for Scientific Technology Promotion, Japan; Nippon Kokan Co., Ltd.; Sumitomo Chemical Co., Ltd.; **Kanto Kagaku** K. K.; Takasago Perfumery Co., Ltd.; Nippon Soda Co., Ltd.; Takeda Chemical Industries, Ltd.
SOURCE: Jpn. Kokai Tokkyo Koho, 13 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 11189600	A2	19990713	JP 1997-359654	19971226
PRIORITY APPLN. INFO.:			JP 1997-359654	1997

OTHER SOURCE(S): CASREACT 131:87713; MARPAT 131:87713
ED Entered STN: 14 Jul 1999
AB Ruthenium-phosphine-amine complexes represented by formula RuXY(PR1R2R3)n(NR6R7R8)m [I; X, Y = H, halo, CO2H, other anion; R1 - R3 = (un)substituted hydrocarbyl; or R1 and R2 are linked together to form an (un)substituted carbocyclic ring; n = 0-4; R6 - R8 = H, (un)substituted hydrocarbyl; m = 0-4], RuXY(PR1R2R3)n(R6R7N-Z-NR9R10)m [II; X, Y, R1 - R3, m = defined in I; R6, R7, R9, R10 = H, (un)substituted hydrocarbyl; Z = (un)substituted hydrocarbyl], RuXY(PR1R2-W-PR4R5)n(NR6R7R8)m [III; X, Y, R6 - R8, n, m = defined in I; R1 - R5 = (un)substituted hydrocarbyl or R1 and R2 or R4 and R5 are linked together to form a (un)substituted carbocyclic ring; W = (un)substituted hydrocarbyl], or RuXY(PR1R2-W-PR4R5)n(R6R7N-Z-NR9R10)m (X, Y, R1 - R5, n, m = defined in III; R6, R7, R9, R10 = defined in II) are prepared Optically active alcs., useful as intermediates for drugs, agrochems., or many commonly used chems., are prepared in high yields and high selectivity by reduction of carbonyl compds. with hydrogen or hydrogen-donating compound in the presence of the above ruthenium-phosphine-amine catalysts. Thus, 534 mg [RuCl2(S)-BINAP](DMF)n, 1.117 mg (S,S)-1,2-diphenylethylenediamine (DPEN), and 15 mL DMF were stirred at room temperature under Ar overnight and cooled to -50°. The precipitated crystals were recrystd. from toluene/hexane to give 361 mg [(S)-BINAP]RuCl2 (S,S)-DPEN (IV). IV (12.2 mg) and 11.5 mg KOCMe3 were dissolved in 5 mL 2-propanol, placed in an autoclave under Ar, and stirred for 30 min. Acetophenone (600 mg) was added and the resulting mixture was pressurized by hydrogen to 3 atm and hydrogeanted under stirring for 50 min to give ≥99% (R)-1-phenethyl alc. of 81.7% ee.
IC ICM C07F015-00
ICS B01J031-24; C07C029-145; C07C033-22; C07B061-00; C07M007-00
CC 25-7 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
Section cross-reference(s): 67, 78

L105 ANSWER 7 OF 18 HCAPLUS COPYRIGHT 2006 ACS on STN DUPLICATE 7
ACCESSION NUMBER: 1999:431891 HCAPLUS
DOCUMENT NUMBER: 131:87717
TITLE: Preparation of alcohols by catalytic hydrogenation of carbonyl compounds
INVENTOR(S): Ikehira, Hideyuki; **Murata, Kunihiko**; **Ikariya, Takao**; Okuma, Takeshi; Noyori, Ryoji
PATENT ASSIGNEE(S): Foundation for Scientific Technology Promotion, Japan; Sumitomo Chemical Co., Ltd.; **Kanto Kagaku** K. K.; Nippon Kokan Co., Ltd.
SOURCE: Jpn. Kokai Tokkyo Koho, 7 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 11189559	A2	19990713	JP 1997-359656	

1997
1226

PRIORITY APPLN. INFO.: JP 1997-359656
1997
1226

OTHER SOURCE(S): CASREACT 131:87717; MARPAT 131:87717

ED Entered STN: 14 Jul 1999

AB Alcs. represented by formula R1CH(OH)R2 [R1, R2 = H, halo, (un)substituted hydrocarbyl or heterocyclyl, RO, RO2C; R = (un)substituted hydrocarbyl or heterocyclyl; or R1 and R2 are linked together to form a ring provided that R1 and R2 are not halogen atoms] are prepared by hydrogenation of carbonyl compds. represented by formula R1COR2 (R1, R2 = same as above) in the presence of a homogeneous hydrogenation catalyst, N-containing organic compound, and base in liquid reaction medium. The homogeneous catalyst is a transition metal catalyst of group VIII metals in particular rhodium, ruthenium, iridium, and platinum, whereas base is an alkali or alkaline earth metal hydroxide or salt or a quaternary ammonium salt. This process uses inexpensive and practical ruthenium complexes of high activity and can rapidly hydrogenate carbonyl compds. to alcs. in high yields which are intermediates for drugs, agrochems., and many commonly used chems. Thus, [RuCl2(cod)]2 0.01, KOH 0.04, ethylenediamine 0.02, and benzophenone 5.0 mmol were dissolved in 10 mL 2-propanol, 2 mL PhMe, and 100 μL DMF and hydrogenated in an 100 mL metal autoclave at hydrogen pressure of 40 atm under stirring for 3 h to give ≥99% benzhydrol (Ph2CHOH).

IC ICM C07C033-18
ICS B01J031-22; C07B041-02; C07C029-145; C07C031-125; C07C035-08; C07B061-00

CC 25-16 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)

L105 ANSWER 8 OF 18 HCAPLUS COPYRIGHT 2006 ACS on STN DUPLICATE 8

ACCESSION NUMBER: 1999:439512 HCAPLUS

DOCUMENT NUMBER: 131:87714

TITLE: Preparation of optical active alcohols by asymmetric hydrogenation of carbonyl compounds

INVENTOR(S): Ikehira, Hideyuki; **Murata, Kunihiko**; **Ikariya, Takao**; Ohkuma, Takeshi; Noyori, Ryoji

PATENT ASSIGNEE(S): Foundation for Scientific Technology Promotion, Japan; Sumitomo Chemical Co., Ltd.; **Kanto Kagaku** K. K.; Nippon Kokan Co., Ltd.

SOURCE: Jpn. Kokai Tokkyo Koho, 8 pp.
CODEN: JKXXAF

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 11189558	A2	19990713	JP 1997-359655	1997 1226

PRIORITY APPLN. INFO.: JP 1997-359655

1997
1226

OTHER SOURCE(S): CASREACT 131:87714; MARPAT 131:87714
ED Entered STN: 19 Jul 1999
AB Optically active alcs. represented by formula R1CHR2OH [R1, R2 = H, halo, (un)substituted hydrocarbyl or heterocyclyl, RO, RO2C; wherein R = (un)substituted hydrocarbyl or heterocyclyl; or R1 and R2 are linked to each other to form a ring constituting an sym. compound] are prepared by stereoselective hydrogenation of carbonyl compds. represented by formula R1COR2 (R1, R2 = same as above) in the presence of a transition metal catalyst, an optically active N-containing compound (in particular optically active amine), and base. This process can also easily recover catalysts in an industrial scale and gives in high yields optically active alcs. of high purity which are useful as liquid crystals or intermediates for drugs. Thus, a 0.5 M KOH solution in 2-propanol (120 μL), 8.5 mg (S,S)-diphenylethylenediamine, 502 mg 2,4'-dichlorobenzophenone, 15 mL 2-propanol, and 4 mL toluene were placed in a reaction tube under Ar, followed by adding 6.1 mg [RuCl2(p-cymene)]2 after degassing-purging with Ar. The resulting solution was repeatedly degassed and purged with Ar, transfered to a metal autoclave and pressurized with hydrogen to 40 atm and stirred at 28° for 4 h to give (+)-2,4'-dichlorobenzhydrol of 45% ee.
IC ICM C07C033-18
ICS B01J031-22; C07B041-02; C07B053-00; C07C029-145; C07C033-46; C07B061-00; C07M007-00
CC 25-7 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)

L105 ANSWER 9 OF 18 HCAPLUS COPYRIGHT 2006 ACS on STN DUPLICATE 9
ACCESSION NUMBER: 1998:115900 HCAPLUS
DOCUMENT NUMBER: 128:154227
TITLE: Preparation of metallocene compounds
INVENTOR(S): Tsutsumi, Kunihiko; Hori, Junichi; Yamazaki, Yasuhiro; Sugawara, Yasuaki; **Murata, Kunihiko**; Yoshida, Masahiro
PATENT ASSIGNEE(S): **Kanto Kagaku**, Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 4 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 10045786	A2	19980217	JP 1996-218089	1996 0801
PRIORITY APPLN. INFO.:			JP 1996-218089	1996 0801

OTHER SOURCE(S): CASREACT 128:154227
ED Entered STN: 26 Feb 1998
AB Characterized is a process for preparation of the title compds. (I) by treatment of cyclopentadiene, indene, fluorene, or bridged compds. thereof with alkyl lithium and reacted with transition metal salts. I, useful as catalysts in the production of polyolefin, are

prepared in an industrial manner efficiently and economically. Thus, 1,1-cyclopentadienyl-(9-fluorenyl)diphenylmethane was treated with n-BuLi in a mixture of toluene and THF, and further reacted with zirconium chloride to give 81% diphenylmethylene (9-fluorenyl) (cyclopentadiene) zirconium chloride.
IC ICM C07F017-00
CC 29-10 (Organometallic and Organometalloidal Compounds)
Section cross-reference(s): 78

L105 ANSWER 10 OF 18 HCAPLUS COPYRIGHT 2006 ACS on STN DUPLICATE 10
ACCESSION NUMBER: 1998:68511 HCAPLUS
DOCUMENT NUMBER: 128:167201
TITLE: Preparation of alkylcyclopentadienes as precursors for hydrogenation and olefin polymerization catalysts
INVENTOR(S): **Murata, Kunihiko**; Tsutsumi, Kunihiko; Yamaguchi, Hiroyuki; Yoshida, Masahiro
PATENT ASSIGNEE(S): **Kanto Kagaku**, Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 5 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 10025258	A2	19980127	JP 1996-200974	19960712
PRIORITY APPLN. INFO.:			JP 1996-200974	19960712

OTHER SOURCE(S): CASREACT 128:167201; MARPAT 128:167201
ED Entered STN: 05 Feb 1998
AB Alkylcyclopentadienes are prepared by reaction of cyclopentadienes with (slightly) ≤1 equivalent mol alkyl lithium and alkylation with RX (R = C1-15 hydrocarbon; X = tosyl, mesyl, halo) in dipolar aprotic solvents. Cyclopentadiene was condensed with BuLi in hexane-THF at room temperature for 3 h and alkylated with BuBr in 1,3-dimethyl-2-imidazolidinone at room temperature for overnight to give 81% n-butylcyclopentadiene (I). I was condensed with BuLi in hexane-toluene at room temperature for 3 h and reacted with ZrCl4 under reflux for 3 h to give 71% dichlorobis(n-butylcyclopentadienyl)zirconium.
IC ICM C07C013-15
ICS C07C002-86; C07C013-465
CC 24-4 (Alicyclic Compounds)
Section cross-reference(s): 35

L105 ANSWER 11 OF 18 HCAPLUS COPYRIGHT 2006 ACS on STN DUPLICATE 11
ACCESSION NUMBER: 1998:228999 HCAPLUS
DOCUMENT NUMBER: 128:270734
TITLE: Transition-metal containing organic compounds and their use as catalysts for olefin polymerization
INVENTOR(S): **Murata, Kunihiko**; Hori, Junichi;

Yoshida, Masahiro
PATENT ASSIGNEE(S): **Kanto Kagaku** K. K., Japan
SOURCE: Eur. Pat. Appl., 12 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 834515	A2	19980408	EP 1997-116930	19970930
EP 834515	A3	19991124		
EP 834515	B1	20040225		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
JP 10109995	A2	19980428	JP 1996-281643	19961004
JP 3566819	B2	20040915		
US 5859276	A	19990112	US 1997-935422	19970923
PRIORITY APPLN. INFO.:			JP 1996-281643 A	19961004

OTHER SOURCE(S): MARPAT 128:270734
ED Entered STN: 23 Apr 1998
AB Metallocene dichlorides were prepared E.g., bis(N-methylanilido)zirconium dichloride-2THF, prepared in 79% yield from PhNHMe and ZrCl4 in THF, was complexed with 1,2-di-3-indenylethane to give 98% ethylenedi-1-indenylzirconium bis(N-methylanilide), which was chlorinated with gaseous HCl in CH2Cl2 to give 62% ethylenedi-1-indenylzirconium dichloride. Similarly prepared was 51% ethylenedi-1-indenylhafnium dichloride.
IC ICM C07F017-00
ICS C08F010-00; C07F007-00
CC 29-10 (Organometallic and Organometalloidal Compounds)

L105 ANSWER 12 OF 18 HCAPLUS COPYRIGHT 2006 ACS on STN DUPLICATE 12
ACCESSION NUMBER: 1998:228998 HCAPLUS
DOCUMENT NUMBER: 128:270733
TITLE: Process for synthesizing metallocene compounds
INVENTOR(S): **Murata, Kunihiko**; Hori, Junichi; Yoshida, Masahiro
PATENT ASSIGNEE(S): **Kanto Kagaku** K. K., Japan
SOURCE: Eur. Pat. Appl., 19 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE

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     EP 834514              A2     19980408    EP 1997-116929
                                                                       1997
                                                                       0930
     EP 834514              A3     19991124
     EP 834514              B1     20031022
         R:  AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE,
             MC, PT, IE, FI
     JP 10109996            A2     19980428    JP 1996-281644
                                                                       1996
                                                                       1004
     JP 3694371             B2     20050914
     US 5892075             A      19990406    US 1997-936169
                                                                       1997
                                                                       0923
PRIORITY APPLN. INFO.:                         JP 1996-281644      A
                                                                       1996
                                                                       1004
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OTHER SOURCE(S): MARPAT 128:270733

ED Entered STN: 23 Apr 1998

AB The object of the invention resides in the development of an improved process for synthesizing metallocene compds. useful as olefin polymerization catalysts. E.g., bis(N-methylanilido)zirconium dichloride-2THF, prepared in 79% yield from PhNHMe and ZrCl4 in THF, was complexed with 1,2-di-3-indenylethane to give 98% ethylenedi-1-indenylzirconium bis(N-methylanilide), which was chlorinated with gaseous HCl in CH2Cl2 to give 62% ethylenedi-1-indenylzirconium dichloride. Similarly prepared was 51% ethylenedi-1-indenylzirconium dichloride.

IC ICM C07F017-00

CC 29-10 (Organometallic and Organometalloidal Compounds)

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=> d l105 13-18 iall abeq tech abex
YOU HAVE REQUESTED DATA FROM FILE 'HCAPLUS, WPIX' - CONTINUE? (Y)/N:y
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L105 ANSWER 13 OF 18  WPIX COPYRIGHT 2006       THE THOMSON CORP on STN
ACCESSION NUMBER:     2005-653595 [67]    WPIX
DOC. NO. CPI:         C2005-197673 [67]
TITLE:                Manufacture of optically active alcohol
                      containing nitrogen-containing heterocyclic ring,
                      involves reacting specific asymmetric metal
                      complex and hydrogen donor
DERWENT CLASS:        B03; C02
INVENTOR:             KATAYAMA T; MURATA K
PATENT ASSIGNEE:      (KAKA-C) KANTO KAGAKU KK
COUNTRY COUNT:        1
```

PATENT INFORMATION:

PATENT NO	KIND	DATE	WEEK	LA	PG	MAIN IPC
JP 2005263662	A	20050929	(200567)*	JA	53[0]	C07D211-14

APPLICATION DETAILS:

PATENT NO	KIND	APPLICATION	DATE

JP 2005263662 A JP 2004-76676 20040317

PRIORITY APPLN. INFO: JP 2004-76676 20040317
INT. PATENT CLASSIF.:
MAIN: C07D211-14
SECONDARY: C07D401-04
BASIC ABSTRACT:

JP 2005263662 A UPAB: 20051223

NOVELTY - An asymmetric metal complex obtained by reacting optically active nitrogen compound, 8th group metallic compound and ketone compound, with salt of nitrogen-containing heteroaromatic compound, is subjected to hydrogen donor reaction, to obtain optically active alcohol containing nitrogen-content heterocyclic ring.

DETAILED DESCRIPTION - An asymmetric metal complex obtained by reacting optically active nitrogen compound of formula (2), 8th group metallic compound and ketone compound, with salt of nitrogen-containing heteroaromatic compound of formula (1), is subjected to hydrogen donor reaction, to obtain optically active alcohol containing nitrogen-content heterocyclic ring of formula (3) and/or (4).

R1-R4=complex monocyclic ring or complex polycyclic groups having saturated or unsaturated optionally substituted aliphatic hydrocarbon, optionally substituted aromatic monocyclic ring or aromatic polynuclear hydrocarbon group or optionally substituted alicyclic hydrocarbon group;

R2=H, halogen, carboxyl group, amino group, amide, hydroxyl, alkoxy or allyloxy;

X-=halogen anion, borate anion, phosphate anion, sulfonate anion or carboxylate anion;

m,n=0-5;

R5=H or optionally substituted alkyl group;and

R6=alkyl group, optionally substituted aromatic monocyclic ring or aromatic polynuclear hydrocarbon group, saturated or unsaturated hydrocarbon or alicyclic hydrocarbon.

USE - As synthetic intermediate, catalyst for asymmetric synthesis, bioactive substance, beta-adrenergic effect blocker, pharmaceutical and agrochemical intermediate.

ADVANTAGE - An optically active alcohol is manufactured by an efficient method.

MANUAL CODE: CPI: B07-D05; B14-J02D2; C07-D05; C14-J02D2; N02-E01

TECH

INORGANIC CHEMISTRY - Preferred Compound: The metallic compound is ruthenium compound.

ORGANIC CHEMISTRY - Preferred Compound: The metallic compound is ruthenium compound.

ORGANIC CHEMISTRY - Preferred Compound: The hydrogen donor is formic acid, formate or alcohol compound. Preferred Method: A base selected from organic amine, alkali metal hydroxide or alkali metal alkoxide, is used as base during manufacture of optically active alcohol.

ABEX DEFINITIONS - Preferred Definitions: - m,n=1; - R1=optionally substituted phenyl preferably 4-cyano phenyl group; - R2=optionally substituted dihydropyridazyl group preferably 4-oxo dihydro pyridazyl group; - R3=group of formula (5); - R4=group of formula (6); - R6=group of formula (7); - R7-R9=H, 1-8C alkyl, halogen atom or 1-8C alkoxy;and - p,q,o=1-5. - R3 and R4 mutually bonds to form a group of formula (8).

SPECIFIC COMPOUNDS - About 300 metallic compounds are disclosed

such as chloro((S,S)-N-(p-toluene sulfonyl)-1,2-diphenyl ethylene diamine) (benzene) ruthenium.

EXAMPLE - 1-(4-cyano phenyl carbonyl methyl)-4-(4,5-dihydropyridazine-3 (2H)-one-6-yl) pyridinium bromide (in g) (3.50), triethyl amine (9.6 ml), formic acid (4.4 ml), asymmetric metal complex (chloro((S,S)-N-(p-toluene sulfonyl)-1,2-diphenyl ethylene diamine) (mesitylene) ruthenium (27.6 mg), were stirred at 40degreesC for 24 hours in a flask. Saturated sodium hydrogen carbonate aqueous solution was added to the reaction liquid. The precipitated powder was filter separated. (R)-6-(1-(2-(4-cyano phenyl)-2-hydroxyethyl)-1,2,5,6-tetrahydro pyrido-4-yl)-4,5-dihydropyridazine-3 (2H)-one of 94% yield and 91% optical purity, was obtained.

L105 ANSWER 14 OF 18 WPIX COPYRIGHT 2006 THE THOMSON CORP on STN
ACCESSION NUMBER: 2004-272579 [26] WPIX
DOC. NO. CPI: C2004-105911 [26]
TITLE: Preparation of aryloxy metallocene compounds such as racemic-ethylene bis(indenyl)zirconium bisphenoxide, useful in polymerization catalyst, involves simple aroxylation reaction
DERWENT CLASS: A17; E11; E12
INVENTOR: HORI J; **MURATA K**
PATENT ASSIGNEE: (KAKA-C) **KANTO KAGAKU KK**
COUNTRY COUNT: 1

PATENT INFORMATION:

PATENT NO	KIND	DATE	WEEK	LA	PG	MAIN IPC
JP 2003231693	A	20030819	(200426)*	JA	19[0]	C07F017-00

APPLICATION DETAILS:

PATENT NO	KIND	APPLICATION	DATE
JP 2003231693	A	JP 2002-26362	20020204

PRIORITY APPLN. INFO: JP 2002-26362 20020204
INT. PATENT CLASSIF.:
MAIN: C07F017-00
SECONDARY: C07F007-00; C07F007-28
BASIC ABSTRACT:

JP 2003231693 A UPAB: 20050528

NOVELTY - An aryloxy metallocene compound such as racemic-ethylene bis(indenyl)zirconium bisphenoxide, racemic-ethylene bis(indenyl)zirconium bis(p-methoxy phenoxide), racemic-ethylene bis(indenyl)zirconium bis(o-phenyl phenoxide) or racemic-ethylene bis(indenyl)zirconium bis(p-methyl phenoxide) is prepared by a simple aroxylation reaction.

DETAILED DESCRIPTION - Preparation of compounds of formula (I) involves reacting compounds of formula (II) and ((III).

L1 and L2 = 1-20C aliphatic hydrocarbon (which may also contain a halogen atom, an oxygen atom, a silicon atom or a germanium atom) or 6-14C aromatic hydrocarbon, cyclopentadienyl, indenyl, tetrahydro indenyl, benzo indenyl, dibenzo indenyl, naphth indenyl, fluorenyl or azulenyl radical optionally joined together through hydrocarbon group, silicon atom or germanium atom;

M = titanium, zirconium or hafnium atom;

X = an oxygen atom or a sulfur atom;
R3-R7 = 1-12C oxygenated organic radical, a hydrogen atom, 1-20C hydrocarbon group, 6-14C aromatic hydrocarbon radical or a halogen atom, or join together to form an aliphatic or aromatic ring.
R1 and R2 = 1-14C aliphatic hydrocarbon or aromatic hydrocarbon radical optionally containing silicon or germanium. R1 and R2 may form a ring containing one or more nitrogen atoms.
USE - The aryloxy metallocene compound is used in polymerization catalysts.
ADVANTAGE - The aryloxy metallocene compound is produced by a cost-effective and simple method. The method avoids use of harmful chemicals which affect environment.

MANUAL CODE: CPI: A02-A06E1; E05-E; E05-E01; E05-F02; E05-L01; E05-M; E05-N

L105 ANSWER 15 OF 18 WPIX COPYRIGHT 2006 THE THOMSON CORP on STN
ACCESSION NUMBER: 2003-868757 [81] WPIX
DOC. NO. CPI: C2003-245785 [81]
TITLE: New optically active diphosphine compound used as catalyst ligand for asymmetric synthesis reactions
DERWENT CLASS: E11; E19; J04
INVENTOR: **IKARIYA T**; **MURATA K**; OTA T; TSUTSUMI K
PATENT ASSIGNEE: (KAKA-C) **KANTO KAGAKU KK**
COUNTRY COUNT: 1

PATENT INFORMATION:

PATENT NO	KIND	DATE	WEEK	LA	PG	MAIN IPC
JP 2003206295	A	20030722	(200381)*	JA	13[0]	C07F009-50

APPLICATION DETAILS:

PATENT NO	KIND	APPLICATION	DATE
JP 2003206295	A	JP 2001-401157	20011228

PRIORITY APPLN. INFO: JP 2001-401157 20011228
INT. PATENT CLASSIF.:
MAIN: C07F009-50
BASIC ABSTRACT:
JP 2003206295 A UPAB: 20050531
NOVELTY - Optically active diphosphine compound (I) is new.
DETAILED DESCRIPTION - An optically active diphosphine compound of formula (I) is new.
R1, R2 = linear or cyclic 1-20C hydrocarbon optionally substituted, preferably methyl or phenyl;
R3, R4 = H or 1-3C hydrocarbon, preferably H; and
R5-R8 = 1-30C hydrocarbon, preferably phenyl, 4-tolyl or 3,5-xylyl.
At least one of R5-R8 is not phenyl.
An INDEPENDENT CLAIM is also included for manufacture of (I).
USE - Ligand for catalyst used in various asymmetric synthesis reactions.
ADVANTAGE - The optically active diphosphine compound

improves the activity of the catalyst. It is obtained efficiently and inexpensively. The manufacturing method has high conversion ratio and selectivity.

MANUAL CODE: CPI: E05-G02; E05-G03B; J04-E04; N05-E01; N06-E01

TECH

ORGANIC CHEMISTRY - Preparation (claimed): Preparation of the optically active diphosphine compound involves producing diaryl phosphine borane by reacting diaryl phosphite and dimethyl sulfide borane.

ABEX DEFINITIONS - Preferred Definitions: - R3 = H; and - R4 = H or methyl.

EXAMPLE - Magnesium (in g) (3.42) and a tetrahydrofuran solution of 5-bromo-m-xylene (25.47) are added to a flask substituted with argon gas. The mixture is stirred at 60 degrees C for 45 minutes. A tetrahydrofuran solution of diethyl phosphite (6 ml) is added in drops for 40 minutes at room temperature. The solution is then refluxed for 3 hours, and the reaction solvent is distilled. Ethyl acetate and hydrochloric acid (150 ml) are added to obtain a saturated salt solution. The salt solution is dried and purified to produce di-(3,5-xylyl) phosphite (A) (10.56). - (A) (2) is dissolved in diethyl ether (20 ml). Dimethyl sulfide borane (0.92) is added and stirred. The reaction solution is filtered, solvent is removed by distillation, and di-(3,5-xylyl) phosphine borane (B) (1.82) is formed. p-Tosyl chloride (3.55), pyridine (1.72 ml), methylene chloride (2 ml) and methylene chloride solution of (R,R)-3-methyl-2,4-pentanediol (5 ml) are reacted at room temperature. Ethyl acetate (60 ml) is added, and a saturated salt solution is obtained after washing. The obtained solution is dried and purified to obtain (S,S)-3-methyl-2,4-pentane di tosylate (C) (1.92). Product (B) (1.82), tetrahydrofuran (12 ml) and n-butyl lithium (4.55 ml) are stirred at room temperature. Subsequently, dimethylformamide solution of product (C) (1.08) and diethyl ether (60 ml) are added to reaction solution and stirred. The saturated salt solution obtained is dried and purified. (S,S)-3-methyl-2,4-bis(di-3,5-xylyl phosphino) pentane (638 mg) is obtained.

L105 ANSWER 16 OF 18 WPIX

ACCESSION NUMBER: 2003-543871 [52] WPIX
DOC. NO. CPI: C2003-147745 [52]
TITLE: New ruthenium complex, used as catalyst for preparing optically active alcohol compound
DERWENT CLASS: E19; J04
INVENTOR: **IKARIYA T**; KUNIHIKO M; KUNIHIKO T; **MURATA K**; OTA T; TAKAO I; TAKESHI O; TSUTSUMI K
PATENT ASSIGNEE: (KAKA-C) **KANTO KAGAKU KK**
COUNTRY COUNT: 33

PATENT INFORMATION:

PATENT NO	KIND	DATE	WEEK	LA	PG	MAIN IPC
EP 1323724	A2	20030702	(200352)*	EN	28[0]	C07F015-00
CA 2414265	A1	20030628	(200353)	EN		C07F015-00
US 20030166978	A1	20030904	(200359)	EN		C07C029-14
JP 2003252884	A	20030910	(200361)	JA	21	C07F009-50
JP 3566955	B2	20040915	(200460)	JA	33	C07F009-50
US 6790973	B2	20040914	(200460)	EN		C07F015-00

APPLICATION DETAILS:

PATENT NO	KIND	APPLICATION	DATE
EP 1323724 A2		EP 2002-28791	20021223
JP 2003252884 A		JP 2002-248058	20020828
JP 3566955 B2		JP 2002-248058	20020828
CA 2414265 A1		CA 2002-2414265	20021216
US 20030166978 A1		US 2002-330501	20021227
US 6790973 B2		US 2002-330501	20021227

FILING DETAILS:

PATENT NO	KIND	PATENT NO
JP 3566955 B2	Previous Publ	JP 2003252884 A

PRIORITY APPLN. INFO: JP 2002-248058 20020828
JP 2001-401170 20011228

INT. PATENT CLASSIF.:
MAIN: C07C029-14; C07F015-00; C07F009-50
SECONDARY: B01J023-46; B01J031-24; C07C213-00; C07C215-30; C07C029-145; C07C031-125; C07C031-135; C07C033-20; C07C033-22; C07C033-46; C07D213-30; C07D307-12; C07D333-16
ADDITIONAL: C07B053-00; C07B061-00
INDEX: C07M007:00

BASIC ABSTRACT:

EP 1323724 A2 UPAB: 20050903

NOVELTY - A ruthenium complex (I) used as catalyst for preparing optically active alcohol compound is new.

DETAILED DESCRIPTION - A ruthenium complex of formula (I) is new:

R1, R2 = 1-20C substituted chain/cyclic hydrocarbon;
R3, R4 = H or 1-3C hydrocarbon;
R5-R8 = 1-30C substituted hydrocarbon; and
X, Y = H or anion.

When X and Y are bromine, R1 and R2 are methyl, and when R3 and R4 are hydrogen, 1 of R5-R8 is not phenyl.

INDEPENDENT CLAIMS are also included for:

(1) a ruthenium complex of formula RuXYAB (II); and

(2) a process for preparing an alcoholic compound comprising reducing a carbonyl compound with reaction of hydrogen or a compound donating hydrogen in presence of (I) or (II).

A = group of formula (III);
B = group of formula (IV);
R9-R16 = H or 1-30 substituted chain/cyclic hydrocarbon; and
Z = 1-10C substituted/single bond chain/cyclic hydrocarbon.

USE - The invention is used as catalyst for preparing optically active alcohol compound (claimed). It is used as intermediate of pharmaceuticals, agricultural chemicals, or commodity chemicals.

ADVANTAGE - The invention has asymmetry on carbon and is easy to synthesize. It provides alcoholic compounds that are excellent in terms of reactivity and enantioselectivity in asymmetric hydrogenation of carbonyl compounds compared with conventional ruthenium complex catalyst.

MANUAL CODE: CPI: E05-G02; E05-G03B; E05-M; E10-E04F; E11-D; J04-E04; N05-B; N05-D; N05-E01; N07-B

TECH
ORGANIC CHEMISTRY - Preferred Compounds: A is TolSKEWPHOS:2,4-bis-(di-4-tolylphosphino)pentane; XylSKEWPHOS:2,4-bis-(di-3,5-xylylphosphino)pentane; 2,4-bis-(diphenylphosphino)-3-methylpentane; 2,4-bis-(di-4-tolylphosphino)-3-methylpentane; 2,4-bis-(di-3,5-xylylphosphino)-3-methylpentane; 1,3-bis-(diphenylphosphino)-1,3-diphenylpropane; 1,3-bis-(di-4-tolylphosphino)-1,3-diphenylpropane; 1,3-bis-(di-3,5-xylylphosphino)-1,3-diphenylpropane; 1,3-bis-(diphenylphosphino)-1,3-diphenyl-2-methylpropane; 1,3-bis-(di-4-tolylphosphino)-1,3-diphenyl-2-methylpropane; or 1,3-bis-(di-3,5-xylylphosphino)1,3-diphenyl-2-methylpropane.
B is diphenylethylenediamine or 1-isopropyl-2,2-di(p-methoxyphenyl)ethylenediamine.
Preferred Method: The complex is obtained by reacting RuXY (V) with compound (III).

ABEX DEFINITIONS - Preferred Definition: - R1, R2 = methyl; - R3, R4 = H; - R5-R8 = phenyl, 4-tolyl, or 3,5-xylyl, preferably phenyl; - R13, R15 = H; - R14, R16 = phenyl; - R13, R14 = isopropyl; - R15, R16 = 4-methoxyphenyl; - R9-R12 = H; and - Z = single bond.
EXAMPLE - (R)-DAIPEN of formula (a) (115 mg, 0.35 mmol) was added to RuBr2((S,S)-Tolskewphos) complex (316 mg, 0.35 mmol) and replaced with argon. Subsequently, the mixture was added with dimethylformamide (14 ml), degassed, and stirred at room temperature overnight. - After the reaction liquid was filtered through a glass filter packed with silica gel, the solvent was evaporated. - The residue was crystallized from methylene chloride/isopropyl ether to give RuBr2((S,S)-Tolskewphos)((R)-daipen) (246 mg, 66% yield). - The formed RuBr2((S,S)-Tolskewphos)((R)-daipen) (2.1 mg (0.002 mmol) was placed in a 100 ml autoclave, replaced with argon, and subsequently added with acetophenone (2.3 ml, 20 mmol), 0.01M KOC(CH3)3-2-propanol solution (8 ml, 0.08 mmol), degassed and replaced with argon. Hydrogen was introduced to a pressure of 9 atm and the reaction was started. - After the reaction mixture was stirred for 19 hours, the reaction pressure was returned to normal pressure, and the quantity and the optical purity of the produced phenylethyl alcohol was determined by gas chromatography on the reaction liquid. - All the reaction substrate was consumed and the yield of product was not less than 99%. Also, for the obtained phenylethyl alcohol, (R)-product was formed in a yield of 93.8%.

L105 ANSWER 17 OF 18 WPIX COPYRIGHT 2006 THE THOMSON CORP on STN
ACCESSION NUMBER: 2000-475385 [41] WPIX
DOC. NO. CPI: C2000-142349 [41]
TITLE: Preparation of alcohol under mild conditions e.g. by hydrogenating carbonyl compound in presence of bipyridyl derivative, transition metal complex and base
DERWENT CLASS: B05; C03; E19
INVENTOR: **IKARIYA T**; IKEHIRA H; KATAYAMA E; KOZAWA M; **MURATA K**; NOYORI R; OHKUMA T; OKUMA T; OZAWA M; YOKOZAWA T
PATENT ASSIGNEE: (NISC-N) JAPAN SCI & TECHNOLOGY CORP; (KAGA-N) KAGAKU GIJUTSU SHINKO JIGYODAN; (KANT-N) KANTA CHEM CO INC; (KAKA-C) **KANTO KAGAKU KK**; (NIPS-C) NIPPON SODA CO; (NISC-C) NISSAN CHEM IND LTD; (SUMO-C) SUMITOMO CHEM CO LTD; (TAKS-C) TAKASAGO INT CORP; (TAKS-C) TAKASAGO PERFUMERY CO LTD

COUNTRY COUNT: 21

PATENT INFORMATION:

PATENT NO	KIND	DATE	WEEK	LA	PG	MAIN IPC
WO 2000035845	A1	20000622	(200041)*	JA	26[0]	C07C029-145
JP 2000178215	A	20000627	(200042)	JA	7	C07C029-145
EP 1142856	A1	20011010	(200167)	EN		C07C029-145
US 6476278	B1	20021105	(200276)	EN		C07C027-00

APPLICATION DETAILS:

PATENT NO	KIND	APPLICATION	DATE
WO 2000035845 A1		WO 1999-JP7035	19991215
JP 2000178215 A		JP 1998-358034	19981216
EP 1142856 A1		EP 1999-959820	19991215
EP 1142856 A1		WO 1999-JP7035	19991215
US 6476278 B1		WO 1999-JP7035	19991215
US 6476278 B1		US 2001-868169	20011025

FILING DETAILS:

PATENT NO	KIND	PATENT NO
EP 1142856 A1	Based on	WO 2000035845 A
US 6476278 B1	Based on	WO 2000035845 A

PRIORITY APPLN. INFO: JP 1998-358034 19981216
INT. PATENT CLASSIF.:
MAIN: C07C027-00; C07C029-145
SECONDARY: B01J031-22; C07C031-10; C07C033-20; C07C033-22; C07C033-30; C07C035-08
ADDITIONAL: C07B061-00
BASIC ABSTRACT:
WO 2000035845 A1 UPAB: 20050411
NOVELTY - Preparation of an alcohol comprises:
(i) reacting a carbonyl compound with hydrogen in the presence of a bipyridyl derivative, Group VIII transition metal complex and base or
(ii) reducing a carbonyl compound in the presence of a bipyridyl derivative, Group VIII transition metal complex, base and alcoholic solvent.
USE - Used for preparing alcohols useful e.g. as intermediates for pharmaceuticals and pesticides.
ADVANTAGE - Process is simple and produces alcohols under mild conditions in high yields with little side product.
MANUAL CODE: CPI: B10-E04; C10-E04; E10-E04D; E10-E04E; E10-E04F

Member(0002)
ABEQ JP 2000178215 A UPAB 20050411
NOVELTY - Preparation of an alcohol comprises:
(i) reacting a carbonyl compound with hydrogen in the presence of a bipyridyl derivative, Group VIII transition metal complex and base or
(ii) reducing a carbonyl compound in the presence of a bipyridyl derivative, Group VIII transition metal complex, base and alcoholic solvent.

USE - Used for preparing alcohols useful e.g. as intermediates for pharmaceuticals and pesticides.

ADVANTAGE - Process is simple and produces alcohols under mild conditions in high yields with little side product.

TECH

ORGANIC CHEMISTRY - Preferred process: Carbonyl compound of formula R1COR2 (I) is reacted in the presence of an alkali metal or alkaline earth metal hydroxide or a quaternary ammonium hydroxide, a metal complex of formula M1XmLn (II) and a bipyridyl compound of formula (III).

R1, R2 = H, halo, alkoxycarbonyl or optionally substituted alkyl, aralkyl, aryl, alkenyl or alkoxy or
R1 + R2 = cyclic group;
M1 = rhodium, ruthenium, iridium or platinum;
X = H, halo, carboxyl, alkoxy or OH;
L = organic group;
m, n = 0-6 and
m + n = 6 or less;
R3-R9 = H, halo or optionally substituted alkyl, aralkylaryl or alkenyl.

ABEX EXAMPLE - Chloro(pentamethylcyclopentadiyl) (1,5-cyclooctanediene) ruthenium (3.8 mg), potassium hydroxide (3.1 mg), 2,2-bipyridyl (3.1 mg) and acetophenone (600.75 mg) in 2-propanol (10 ml) were heated in an autoclave under hydrogen at 28degreesC and 50 atmospheres pressure for 3 hours with stirring to give 1-phenolethanol in at least 99% yield. In a comparative example in the absence of bipyridyl, the yield was 97% with 3% impurities.

L105 ANSWER 18 OF 18 WPIX COPYRIGHT 2006 THE THOMSON CORP on STN

ACCESSION NUMBER:	1991-278290 [38] WPIX
DOC. NO. CPI:	C1991-120791 [21]
TITLE:	Optically active fluoro-alcohol(s) - useful as intermediates for pharmaceuticals, agrochemicals or liquid crystals
DERWENT CLASS:	B05; C03; E16
INVENTOR:	FUJII T; FUKIAGE A; **MURATA K**; YOSHIDA M
PATENT ASSIGNEE:	(KAKA-C) **KANTO KAGAKU KK**
COUNTRY COUNT:	1

PATENT INFORMATION:

PATENT NO	KIND	DATE	WEEK	LA	PG	MAIN IPC
JP 03184929	A	19910812	(199138)*	JA		
JP 2879456	B2	19990405	(199919)	JA	9	C07C031-38

APPLICATION DETAILS:

PATENT NO	KIND	APPLICATION	DATE
JP 03184929	A	JP 1989-323851	19891215
JP 2879456	B2	JP 1989-323851	19891215

FILING DETAILS:

PATENT NO	KIND	PATENT NO
JP 2879456 B2	Previous Publ	JP 03184929 A

PRIORITY APPLN. INFO: JP 1989-323851 19891215
INT. PATENT CLASSIF.:
MAIN: C07C031-38
SECONDARY: C07C029-40
ADDITIONAL: B01J031-02; C07B061-00
BASIC ABSTRACT:
JP 03184929 A UPAB: 20050502
Optically active fluoro-alcohols (I) are new. In (I), R1 = 1-18C alkyl; R2 = 1-18C alkyl; asterisk C = asymmetric carbon atom.
Production of (I) comprises reacting a fluoro-aldehyde R1-CHF-CH=O (II) with an organometallic reagent as an alkylating agent in the presence or absence of a catalyst. Examples of the organometallic reagents are alkyl magnesium, alkyl lithium, alkyl titanium, alkyl lead and alkyl zinc.
USE/ADVANTAGE - (I) is useful as an intermediate for pharmaceuticals, agrochemicals or functional materials (e.g. strong dielectric liquid crystals). @(9pp Dwg.No.0/0)@
MANUAL CODE: CPI: B10-E04D; B11-B; C10-E04D; C11-B; E10-E04F; N06

Member(0002)
ABEQ JP 2879456 B2 UPAB 20050502
Optically active fluoro-alcohols (I) are new. In (I), R1 = 1-18C alkyl; R2 = 1-18C alkyl; asterisk C = asymmetric carbon atom. Prodn. of (I) comprises reacting a fluoro-aldehyde R1-CHF-CH=O (II) with an organometallic reagent as an alkylating agent in the presence or absence of a catalyst. Examples of the organometallic reagents are alkyl magnesium, alkyl lithium, alkyl titanium, alkyl lead and alkyl zinc.
USE/ADVANTAGE - (I) is useful as an intermediate for pharmaceuticals, agrochemicals or functional materials (e.g. strong dielectric liquid crystals).

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     (FILE 'HOME' ENTERED AT 09:16:37 ON 21 NOV 2006)

     FILE 'HCAPLUS' ENTERED AT 09:17:08 ON 21 NOV 2006
                E US20040176616/PN
L1            1 SEA ABB=ON  PLU=ON  US20040176616/PN
                D ALL
                SEL RN

     FILE 'REGISTRY' ENTERED AT 09:19:43 ON 21 NOV 2006
L2           33 SEA ABB=ON  PLU=ON  (105-45-3/BI OR 105-53-3/BI OR
                108-59-8/BI OR 1121-66-0/BI OR 126-39-6/BI OR 151600-50
                -9/BI OR 154194-50-0/BI OR 160115-23-1/BI OR 164931-77-
                5/BI OR 164931-78-6/BI OR 167316-27-0/BI OR 173837-41-7
                /BI OR 188444-42-0/BI OR 193530-87-9/BI OR 194095-90-4/
                BI OR 22748-16-9/BI OR 24347-58-8/BI OR 287493-81-6/BI
                OR 287493-82-7/BI OR 568590-07-8/BI OR 569342-29-6/BI
                OR 609-02-9/BI OR 67421-02-7/BI OR 724774-82-7/BI OR
                724774-83-8/BI OR 724774-84-9/BI OR 725737-67-7/BI OR
                725737-68-8/BI OR 725737-69-9/BI OR 725737-70-2/BI OR
                725737-71-3/BI OR 930-30-3/BI OR 930-68-7/BI)
                D SCAN

     FILE 'STNGUIDE' ENTERED AT 09:20:12 ON 21 NOV 2006

     FILE 'REGISTRY' ENTERED AT 09:45:35 ON 21 NOV 2006
L3            9 SEA ABB=ON  PLU=ON  L2 AND ?CYCLOPENT?/CNS
                D SCAN
                D 1-9 RN CN STR
L4            1 SEA ABB=ON  PLU=ON  194095-90-4/RN
                D SCAN
                D CN
                E "(+)-(R)-3-[BIS(METHOXYCARBONYL)METHYL]CYCLOPENTANONE
                E "(+)-(R)-3-(BIS(METHOXYCARBONYL)METHYL)CYCLOPENTANONE
                E "(+)-(R)-3-(BIS(ETHOXYCARBONYL)METHYL)CYCLOPENTANONE"
                E "(+)-(R)-3-(BIS(METHOXYCARBONYL)METHYL)CYCLOPENTANONE
L5            1 SEA ABB=ON  PLU=ON  "(+)-(R)-3-(BIS(METHOXYCARBONYL)MET
                HYL)CYCLOPENTANONE"/CN
                D SCAN
                E "PROPANEDIOIC ACID, [(1R)-3-OXOCYCLOPENTYL]-, DIETHYL
                D SCAN L3
                D SCAN L4
L6            2 SEA ABB=ON  PLU=ON  L3 AND ?DIETHYL?/CNS
                D SCAN
L7            1 SEA ABB=ON  PLU=ON  193530-87-9/RN
                D SCAN
                D CN
                E HEXAMETHYLENE BENZENE/CN

     FILE 'LREGISTRY' ENTERED AT 10:09:58 ON 21 NOV 2006
L8              STR

     FILE 'REGISTRY' ENTERED AT 10:23:29 ON 21 NOV 2006
L9           28 SEA SSS SAM L8

     FILE 'CASREACT' ENTERED AT 10:24:16 ON 21 NOV 2006
L10             STR L8
L11           5 SEA SSS SAM L10 (    37 REACTIONS)
                D SCAN
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     FILE 'REGISTRY' ENTERED AT 10:35:31 ON 21 NOV 2006
L12            6 SEA ABB=ON  PLU=ON  L2 AND 1/M
                 D SCAN

     FILE 'CASREACT' ENTERED AT 10:38:21 ON 21 NOV 2006
L13              STR L10
L14            1 SEA SSS SAM L13 (     14 REACTIONS)
                 D SCAN
L15          629 SEA SSS FUL L10 (   2897 REACTIONS)
                 SAV L15 SHI806CASRCT/A
L16          266 SEA ABB=ON  PLU=ON  L15 AND L2
                 D SCAN L14
                 D QUE L14
                 D QUE STAT
                 D QUE STAT L14
L17              STR L13
L18            1 SEA SSS SAM L17 (     14 REACTIONS)
                 D SCAN
L19            1 SEA SUB=L15 SSS SAM L17 (     14 REACTIONS)
                 D SCAN
L20            7 SEA SUB=L15 SSS FUL L17 (     31 REACTIONS)
                 D SCAN
                 D QUE STAT
                 SAV TEMP L20 SHI806CSRCTA/A

     FILE 'ZCAPLUS' ENTERED AT 10:57:30 ON 21 NOV 2006

     FILE 'HCAPLUS' ENTERED AT 12:31:02 ON 21 NOV 2006
                 D SCAN L1

     FILE 'ZCAPLUS' ENTERED AT 12:31:02 ON 21 NOV 2006
                 D QUE STAT L9

     FILE 'REGISTRY' ENTERED AT 12:40:02 ON 21 NOV 2006
L21              SCR 1918 OR 2043 OR 1840 OR 1949 OR 2010
L22           30 SEA SSS SAM L8 NOT L21
                 D QUE STAT

     FILE 'LREGISTRY' ENTERED AT 12:42:18 ON 21 NOV 2006
L23              STR L8

     FILE 'REGISTRY' ENTERED AT 12:43:54 ON 21 NOV 2006
L24           19 SEA SSS SAM L23 NOT L21
                 D SCAN
                 D QUE

     FILE 'LREGISTRY' ENTERED AT 12:46:30 ON 21 NOV 2006

     FILE 'STNGUIDE' ENTERED AT 12:49:12 ON 21 NOV 2006
                 D QUE STAT
                 D COST

     FILE 'LREGISTRY' ENTERED AT 12:55:04 ON 21 NOV 2006
L25              STR L23

     FILE 'REGISTRY' ENTERED AT 12:57:18 ON 21 NOV 2006
L26           47 SEA SSS SAM L25 NOT L21
                 D QUE STAT
L27        12118 SEA SSS FUL L25 NOT L21
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L28          15 SEA ABB=ON  PLU=ON  L2 AND L27
                SAV TEMP L27 SHI806REG/A
                D SAV
L29          18 SEA ABB=ON  PLU=ON  L2 NOT L28
                D SCAN

     FILE 'LREGISTRY' ENTERED AT 13:03:24 ON 21 NOV 2006
L30             STR L25

     FILE 'REGISTRY' ENTERED AT 13:10:40 ON 21 NOV 2006
L31          50 SEA SUB=L27 SSS SAM L30
L32        2503 SEA SUB=L27 SSS FUL L30
                SAV TEMP L27 SHI806REGA/A
                D QUE STAT
L33          14 SEA ABB=ON  PLU=ON  L2 AND L32
                D SCAN
                D QUE STAT

     FILE 'LREGISTRY' ENTERED AT 13:14:01 ON 21 NOV 2006

     FILE 'HCAPLUS' ENTERED AT 13:14:32 ON 21 NOV 2006
                D SCAN L1

     FILE 'LREGISTRY' ENTERED AT 13:14:32 ON 21 NOV 2006
L34             STR L30

     FILE 'REGISTRY' ENTERED AT 13:17:50 ON 21 NOV 2006
L35          50 SEA SSS SAM L34
L36          50 SEA SSS SAM L34 NOT L21

     FILE 'LREGISTRY' ENTERED AT 13:19:08 ON 21 NOV 2006
L37             STR

     FILE 'REGISTRY' ENTERED AT 13:24:03 ON 21 NOV 2006
L38             SCR 1918 OR 2043 OR 1839 OR 1945 OR 2005
L39          50 SEA SSS SAM L37 NOT L38
L40             SCR 1918 OR 2043 OR 1839 OR 1944 OR 2005
L41          50 SEA SSS SAM L37 NOT L40
L42        6815 SEA SSS FUL L37 NOT L40
                SAV TEMP L42 SHI806REGB/A

     FILE 'HCAPLUS' ENTERED AT 13:30:04 ON 21 NOV 2006

     FILE 'REGISTRY' ENTERED AT 13:30:23 ON 21 NOV 2006
L43           4 SEA ABB=ON  PLU=ON  L2 AND L42
                D SCAN

     FILE 'HCAPLUS' ENTERED AT 13:31:18 ON 21 NOV 2006
L44          52 SEA ABB=ON  PLU=ON  L28
L45        6470 SEA ABB=ON  PLU=ON  L43
L46          49 SEA ABB=ON  PLU=ON  L44 AND L45
L47          50 SEA ABB=ON  PLU=ON  L28/P
L48        4494 SEA ABB=ON  PLU=ON  L43/RACT
L49          47 SEA ABB=ON  PLU=ON  L48 AND L47
L50        1507 SEA ABB=ON  PLU=ON  L32/P
L51       31232 SEA ABB=ON  PLU=ON  L42/RACT
L52         266 SEA ABB=ON  PLU=ON  L50 AND L51
                D SCAN L1
                E ASYMMETRIC SYNTHESIS AND INDUCTION/CT
                E E3+ALL
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                E "ASYMMETRIC SYNTHESIS AND INDUCTION"+PFT,OLD,NT/CT
L53             QUE ABB=ON  PLU=ON  "ASYMMETRIC SYNTHESIS AND INDUCTION
                "+PFT,OLD,NT/CT
                E MICHAEL REACTION/CT
                E E3+ALL
L54             QUE ABB=ON  PLU=ON  "MICHAEL REACTION"+PFT,OLD,NT/CT
                E MICHAEL REACTION CATALYSTS/CT
                E E3+ALL
L55             QUE ABB=ON  PLU=ON  "MICHAEL REACTION CATALYSTS"+PFT,OL
                D,NT/CT
L56          30 SEA ABB=ON  PLU=ON  L53 AND L52
L57          21 SEA ABB=ON  PLU=ON  L56 AND (L54 OR L55)
                D SCAN
L58           1 SEA ABB=ON  PLU=ON  L1 AND L57
L59        5174 SEA ABB=ON  PLU=ON  L27/P
L60       31232 SEA ABB=ON  PLU=ON  L42/RACT
L61        1337 SEA ABB=ON  PLU=ON  L60 AND L53
L62         176 SEA ABB=ON  PLU=ON  L61 AND (L54 OR L55)
L63          92 SEA ABB=ON  PLU=ON  L62 AND L55

     FILE 'REGISTRY' ENTERED AT 13:44:20 ON 21 NOV 2006
L64      744935 SEA ABB=ON  PLU=ON  ((FE OR CO OR NI OR RU OR RH OR PD
                OR OS OR IR OR PT)(L)N)/ELS
L65           6 SEA ABB=ON  PLU=ON  L2 AND L64
                D SCAN
L66      316118 SEA ABB=ON  PLU=ON  L64 AND 1-2/N
L67      262888 SEA ABB=ON  PLU=ON  L66 AND 1/M
L68       22790 SEA ABB=ON  PLU=ON  L67 AND 1/RU
L69       80253 SEA ABB=ON  PLU=ON  L67 AND (1/OS OR 1/IR OR 1/PT OR
                1/PD)
L70      159878 SEA ABB=ON  PLU=ON  L67 NOT (L68 OR L69)
L71       76518 SEA ABB=ON  PLU=ON  L70 AND 1/FE
                SET DETAIL ON PERM
L72       83360 SEA ABB=ON  PLU=ON  L67 NOT (L68 OR L69 OR L71)

     FILE 'HCAPLUS' ENTERED AT 14:06:41 ON 21 NOV 2006
L73             QUE ABB=ON  PLU=ON  L68
L74             QUE ABB=ON  PLU=ON  L69
L75             QUE ABB=ON  PLU=ON  L71
L76             QUE ABB=ON  PLU=ON  L72
L77             QUE ABB=ON  PLU=ON  L73 OR L74 OR L75 OR L76
L78          10 SEA ABB=ON  PLU=ON  L63 AND L77
L79           1 SEA ABB=ON  PLU=ON  L1 AND L78
                D QUE
L80        9613 SEA ABB=ON  PLU=ON  L27
L81       50879 SEA ABB=ON  PLU=ON  L42
                D QUE
L82          31 SEA ABB=ON  PLU=ON  L80 AND L81 AND L77
                D QUE
L83           7 SEA ABB=ON  PLU=ON  L82 AND L53
                D QUE
                D QUE L32
L84        1971 SEA ABB=ON  PLU=ON  L32
L85         315 SEA ABB=ON  PLU=ON  L84 AND L42
L86          14 SEA ABB=ON  PLU=ON  L85 AND L77

     FILE 'STNGUIDE' ENTERED AT 14:21:41 ON 21 NOV 2006

     FILE 'HCAPLUS' ENTERED AT 14:21:47 ON 21 NOV 2006
                D SCAN
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     FILE 'STNGUIDE' ENTERED AT 14:22:02 ON 21 NOV 2006
                D QUE STAT

     FILE 'REGISTRY' ENTERED AT 14:25:13 ON 21 NOV 2006

     FILE 'HCAPLUS' ENTERED AT 14:25:15 ON 21 NOV 2006
L87          39 SEA ABB=ON  PLU=ON  L57 OR L78 OR L83 OR L86
L88           1 SEA ABB=ON  PLU=ON  L1 AND L87
                D SCAN L87

     FILE 'STNGUIDE' ENTERED AT 14:27:48 ON 21 NOV 2006

     FILE 'HCAPLUS' ENTERED AT 14:30:37 ON 21 NOV 2006
L89          62 SEA ABB=ON  PLU=ON  L87 OR L56 OR L82
L90          48 SEA ABB=ON  PLU=ON  L89 AND (L53 OR L54 OR L55)
L91           1 SEA ABB=ON  PLU=ON  L1 AND L90

     FILE 'ZCAPLUS' ENTERED AT 14:32:11 ON 21 NOV 2006
L92             QUE ABB=ON  PLU=ON  PY<2005 OR PRY<2005 OR AY<2005 OR
                MY<2005 OR REVIEW/DT

     FILE 'HCAPLUS' ENTERED AT 14:39:30 ON 21 NOV 2006
L93          34 SEA ABB=ON  PLU=ON  L90 AND L92
                D SCAN TI CC

     FILE 'STNGUIDE' ENTERED AT 14:40:51 ON 21 NOV 2006

     FILE 'HCAPLUS' ENTERED AT 14:41:26 ON 21 NOV 2006
                D SCAN
L94          15 SEA ABB=ON  PLU=ON  L93 AND L53 AND L54 AND L55
L95           1 SEA ABB=ON  PLU=ON  L1 AND L94
                D SCAN
                D SCAN L94
L96          34 SEA ABB=ON  PLU=ON  L93 OR L94
L97             QUE ABB=ON  PLU=ON  (KANTO(W)KAGAKU?)/PA,CS,CO,SO
L98             QUE ABB=ON  PLU=ON  WATANABE M?/AU OR MURATA K?/AU OR
                IKARIYA T?/AU
L99          12 SEA ABB=ON  PLU=ON  L97 AND L98
                D SCAN
                D SAV
                SAV TEMP L96 SHI806HCP/A
                SAV TEMP L99 SHI806HCPIN/A

     FILE 'MEDLINE' ENTERED AT 14:56:18 ON 21 NOV 2006
L100          0 SEA ABB=ON  PLU=ON  L97 AND L98

     FILE 'EMBASE' ENTERED AT 15:04:58 ON 21 NOV 2006
L101          0 SEA ABB=ON  PLU=ON  L97 AND L98

     FILE 'BIOSIS' ENTERED AT 15:05:14 ON 21 NOV 2006
L102          0 SEA ABB=ON  PLU=ON  L97 AND L98

     FILE 'WPIX, CONFSCI, PASCAL, TEMA, JICST-EPLUS, NTIS, JAPIO,
     SCISEARCH' ENTERED AT 15:06:47 ON 21 NOV 2006
L103         18 SEA ABB=ON  PLU=ON  L97 AND L98
                SET DETAIL ON PERM
L104         18 SEA ABB=ON  PLU=ON  L97 AND L98
                D TRI 1-18
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     FILE 'HCAPLUS, WPIX' ENTERED AT 15:09:37 ON 21 NOV 2006
L105           18 DUP REM L99 L104 (12 DUPLICATES REMOVED)
                  ANSWERS '1-12' FROM FILE HCAPLUS
                  ANSWERS '13-18' FROM FILE WPIX

     FILE 'HCAPLUS' ENTERED AT 15:10:33 ON 21 NOV 2006

     FILE 'CAOLD' ENTERED AT 15:10:44 ON 21 NOV 2006
L106          816 SEA ABB=ON  PLU=ON  L27
L107          175 SEA ABB=ON  PLU=ON  L32
L108         1649 SEA ABB=ON  PLU=ON  L42
L109           21 SEA ABB=ON  PLU=ON  L106 AND L108
L110            6 SEA ABB=ON  PLU=ON  L108 AND L107
                D SCAN L110
L111           21 SEA ABB=ON  PLU=ON  L109 OR L110
L112          120 SEA ABB=ON  PLU=ON  L68
L113            0 SEA ABB=ON  PLU=ON  L112 AND L111

     FILE 'CASREACT' ENTERED AT 15:19:13 ON 21 NOV 2006
                D QUE STAT L20
                D QUE STAT L20
                D QUE STAT L20
                D L20 1-7 IALL HIT

     FILE 'HCAPLUS' ENTERED AT 15:32:12 ON 21 NOV 2006
                D QUE STAT L93
                D L93 1-34 IBIB ABS ED HITSTR HITIND

     FILE 'CAOLD' ENTERED AT 15:35:33 ON 21 NOV 2006
                D QUE STAT L111
                D QUE L111
                D L111 1-21 IALL HITSTR HITIND
                D QUE STAT L99
                D QUE STAT L104
                D QUE STAT L105

     FILE 'HCAPLUS, WPIX' ENTERED AT 15:42:35 ON 21 NOV 2006
                D L105 1-12 IBIB ED AB HITIND

     FILE 'CAOLD' ENTERED AT 15:42:38 ON 21 NOV 2006

     FILE 'HCAPLUS, WPIX' ENTERED AT 15:44:05 ON 21 NOV 2006
                D L105 13-18 IALL ABEQ TECH ABEX

     FILE 'CAOLD' ENTERED AT 15:44:10 ON 21 NOV 2006


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